

## Supporting Information

### Metal Free Oxidative Decarbonylative Halogenation of Fused imidazoles

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## 1. General information.

All reactions were carried out using pre-dried reaction tube. Commercially available chemicals were purchased from Sigma-Aldrich and Alfa Aesar Pvt. Ltd., India. These chemicals were used without further purification. Progress of the reactions was monitored by thin-layer chromatography (TLC) plates visualized by UV light, I<sub>2</sub> and by treating the plates with dragendorff reagent followed by heating. Silica-gel column chromatography (100–200 mesh) was used for purification. <sup>1</sup>H and <sup>13</sup>C NMR spectra were recorded on Bruker-Avance DPX FT-NMR 500 and 400 MHz instruments. Chemical data for protons are reported in parts per million (ppm) downfield from tetramethylsilane and are referenced to the residual proton in the NMR solvent (CDCl<sub>3</sub>: 7.26 ppm). Carbon nuclear magnetic resonance spectra (<sup>13</sup>C NMR solvent CDCl<sub>3</sub>: 77.0 ppm) were recorded at 125 MHz or 100 MHz. Signal multiplicity is expressed as follows: s (singlet), brs (broad singlet), d (doublet), t (triplet), q (quartet), m (multiplet). J values are given in hertz (Hz). Mass spectra were obtained using Q-TOF-HR/MS spectrometer using electron spray ionization.

## 2. General experimental procedure for the synthesis of starting compounds

### 2.1 Synthetic scheme and procedure for the synthesis of 2-Phenylimidazo[1,2-a]pyridine-3-carbaldehyde (1)

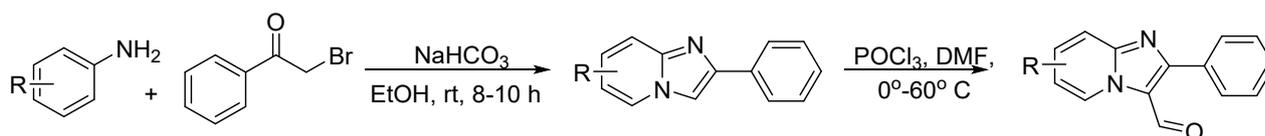
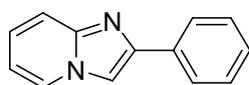
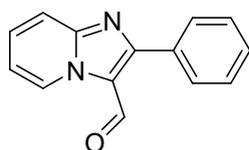


Fig.1. Synthesis of 2-phenylimidazo[1,2-a]pyridine-3-carbaldehyde



**2-Phenylimidazo[1,2-a]pyridine**<sup>[1]</sup>: 2-aminopyridine (10 mmol) and phenacyl bromide (10 mmol) were dissolved in 20 mL ethanol after in a 50 mL round bottom flask. After that sodium bicarbonate (12 mmol) was added to the above solution with stirring. The reaction mixture was continued stirred at room temperature for 8-10 h, and the progress of reaction was monitored by TLC. After completion of the reaction, ethanol was evaporated by rotavapor. The resulting mixture was quenched by adding 10 mL water and extracted with CH<sub>2</sub>Cl<sub>2</sub> (3 × 20 mL) and combined organic layers were washed with brine (20 mL), dried over Na<sub>2</sub>SO<sub>4</sub> and concentrated under reduced pressure. The residue was purified by column chromatography [silica gel, 5% methanol in methylene chloride] to yield desired product (1.746 g, 90% yield). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.11 (d, *J* = 6.7 Hz, 1H), 7.96 (d, *J* = 7.3 Hz, 2H), 7.86 (s, 1H), 7.64 (d, *J* = 9.1 Hz, 1H), 7.44 (t, *J* = 7.6 Hz, 2H), 7.33 (t, *J* = 7.3 Hz, 1H), 7.19 – 7.13 (m, 1H), 6.79-6.77 (m, *J* = 6.6 Hz, 1H).



**2-Phenylimidazo[1,2-a]pyridine-3-carbaldehyde**<sup>[2]</sup>: In a stirred solution of 2-phenylimidazo [1, 2-a]pyridine (5 mmol) in 5 mL DMF at 0°C, POCl<sub>3</sub> (0.92 mL, 10 mmol) was added dropwise. The reaction mixture was kept at 0 °C for half an hour and then the reaction mixture heated at 60 °C for 3 h. Completion of the reaction was monitored by TLC. After completion, the reaction mixture was cooled and quenched with ice. The reaction mixture was extracted with EtOAc (3 x 20 mL), combined organic layer was washed with brine, dried over anhydrous Na<sub>2</sub>SO<sub>4</sub> and concentrated under reduced pressure. The crude product was purified by column chromatography (silica gel, EtOAc in hexane) to obtain the pure product (0.984g, 86% yield). <sup>1</sup>H NMR (400

MHz, CDCl<sub>3</sub>) δ 10.08 (s, 1H), 9.67 (d, J = 6.8 Hz, 1H), 7.85 (d, J = 2.5 Hz, 1H), 7.82 (d, J = 8.5 Hz, 2H), 7.62 – 7.56 (m, 1H), 7.54 (d, J = 6.9 Hz, 3H), 7.14 (t, J = 6.7 Hz, 1H).

## 2.2. Synthetic scheme and procedure for the synthesis of 2-phenylbenzo[d]imidazo[2,1-b]thiazole-3-carbaldehyde (5)

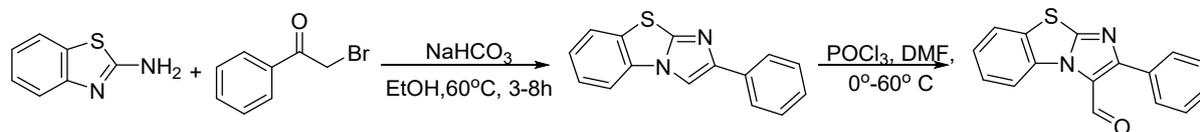
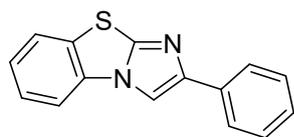


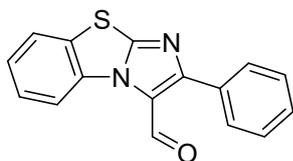
Fig.2. Synthesis of 2-phenylbenzo[d]imidazo[2,1-b]thiazole-3-carbaldehyde

### 2-Phenylbenzo[d]imidazo[2,1-b]thiazole<sup>[3]</sup>:



In a 50 mL round bottom flask, 2-aminobenzothiazole (1g, 6.7 mmol, 1.0 equiv.) and 2-bromo acetophenone (1.592g, 8.3 mmol, 1.2 equiv.) were dissolved into 20 mL of ethanol. The reaction mixture was stirred at 60° C. After completion of the reaction as monitored by TLC, the reaction mixture was cooled, concentrated under reduced pressure and extracted with EtOAc (3 x 25 mL). The combined organic layer was washed with brine, dried over anhydrous Na<sub>2</sub>SO<sub>4</sub> and concentrated under reduced pressure. The crude product was purified by column chromatography using silica gel, EtOAc in hexane to obtain pure benzo[d]imidazo[2,1-b]thiazole in (1.507 g, 90% yield).

### 2-Phenylbenzo[d]imidazo[2,1-b]thiazole-3-carbaldehyde<sup>[4]</sup>:



To a stirred solution of 2-phenylbenzo[d]imidazo[2,1-b]thiazole (1.1g, 4.4 mmol) in 5 mL DMF at 0 °C in 50 mL two-neck round bottom flask, POCl<sub>3</sub> (0.820 mL, 8.8 mmol) was added dropwise. Initially, the reaction mixture was stirred at 0°C for 15 minutes and then heated at 60 °C for 4 h. After completion of reaction (completion of the reaction was monitored by TLC), the reaction mixture was cooled, quenched with ice and extracted with EtOAc (3 x 20 mL). The combined organic layer was washed with brine, dried over anhydrous Na<sub>2</sub>SO<sub>4</sub> and concentrated under reduced pressure. The crude product was purified by column chromatography (silica gel, EtOAc in hexane) to obtain the pure product (0.978g, 80% yield); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 9.86 (s, 1H), 9.22 – 9.18 (m, 1H), 7.78 – 7.71 (m, 3H), 7.56 – 7.50 (m, 4H), 7.45 – 7.40 (m, 1H).

## 2.3. Synthetic scheme and procedure for the synthesis of N-protected benzimidazole-2-carbaldehyde (7)

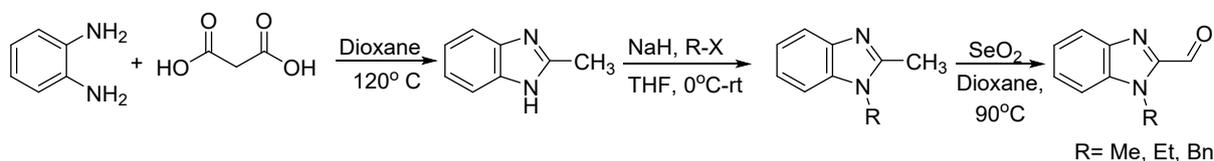
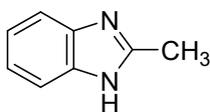


Fig. 3. Synthesis of N-protected benzimidazole-2-carbaldehyde

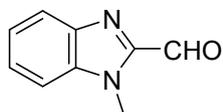
### 2-Methyl-1H-benzo[d]imidazole<sup>[5]</sup>:



In an oven dried sealed tube, a mixture of 1,2-phenylenediamine (500 mg, 4.6 mmol) and malonic acid (2.4 g, 23 mmol) was dissolved in 10 ml of 1,4-dioxane and heated at 120°C on magnetic stirrer for 10 hours. On completion of reaction as monitored by TLC, the reaction mixture was neutralised using saturated sodium bicarbonate solution (20 mL) and organic part was

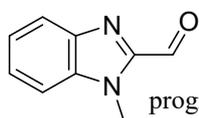
extracted with ethyl acetate (3 x 20 mL). The combined organic layer was washed with brine solution, dried over Na<sub>2</sub>SO<sub>4</sub> and concentrated under reduced pressure. The crude product was purified by column chromatography (silica gel, 0-5% methanol in DCM) to obtain 2-methyl-1H-benzimidazole as white solid (460 mg, 75% yield). NMR data of the product was compared with literature.

#### 1-Methyl-2-methyl-1H-benzo[d]imidazole<sup>[6]</sup>:



To a solution of 2-methyl-1H-benzo[d]imidazole (400 mg, 3.0 mmol) in THF (5 mL) at 0°C, sodium hydride (180 mg, 4.5 mmol) was added portion wise. After stirring for 15 minutes, methyl iodide solution (2.0 M in tert-butyl methyl ether, 521 mg, 3.69 mmol) was slowly added. The reaction was allowed to warm up to rt and stirred until the completion of reaction as monitored by depletion of starting benzimidazole (2–3 hours). The reaction was then quenched with water, extracted with EtOAc (3 x 15 mL) and dried over Na<sub>2</sub>SO<sub>4</sub>. The combined organic layer was concentrated under reduced pressure and purified using silica gel chromatography (0-5% methanol in DCM as eluent) to afford the corresponding alkylated benzimidazole (350 mg, 79% yield).

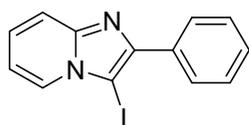
#### 1-Methyl-1H-benzo[d]imidazole-2-carbaldehyde:



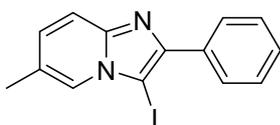
1-methyl-2-methyl-1H-benzo[d]imidazole (350 mg, 2.39 mmol), selenium dioxide (527 mg, 4.79 mmol) was stirred at 85° C in a 50 mL round bottom flask. After 8 hr (reaction progress was monitored by TLC), the reaction mixture was filtered through a small bed of Celite and concentrated under reduced pressure. The crude product is purified through column chromatography using silica gel, methanol in DCM to afford pure product (205 mg, 53% yield); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 10.13 (s, 1H), 7.93 (d, J = 8.2 Hz, 1H), 7.49 (d, J = 4.3 Hz, 2H), 7.41 (ddd, J = 8.1, 5.2, 3.0 Hz, 1H), 4.17 (s, 3H).

### 3. Typical experimental procedure for the synthesis of final compounds

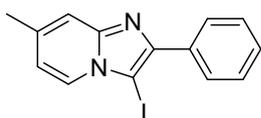
#### 3.1. Typical procedure for the synthesis of 3-iodo-2-phenylimidazo[1,2-a]pyridine (2a) :



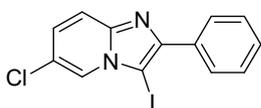
To a stirred solution of 2-phenylimidazo[1,2-a]pyridine-3-carbaldehyde **1a** (111 mg, 0.5 mmol) in acetonitrile (3 mL), TBHP (70 % in water, 192 μL, 1.5 mmol) and molecular iodine (127 mg, 0.5 mmol) were added. The mixture was heated at 60°C for 3 h (monitored by TLC). After completion, the reaction mixture was cooled to room temperature and saturated sodium thiosulfate solution was added. The organic layer was extracted with EtOAc (10x3 ml), dried over anhydrous Na<sub>2</sub>SO<sub>4</sub> and concentrated under reduced pressure. The crude residue was purified by silica gel column chromatography (EtOAc/n-hexane = 1:9) to afford compound **2a** as an off white solid (131 mg, 82% yield); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.25 (d, J = 6.7 Hz, 1H), 8.07 (d, J = 7.4 Hz, 2H), 7.68 (d, J = 8.9 Hz, 1H), 7.51-7.48 (m, 2H), 7.43 – 7.39 (m, 1H), 7.32 – 7.28 (m, 1H), 6.98-6.95 (m, 1H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 147.93, 147.77, 133.22, 128.58, 128.50, 128.43, 126.62, 125.92, 117.53, 113.42, 59.65; ESI-LCMS (m/z): calcd for C<sub>13</sub>H<sub>10</sub>IN<sub>2</sub> [M + H]<sup>+</sup>, 320.98; found, 321.03.



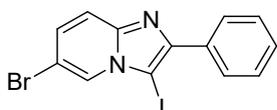
**3-Iodo-6-methyl-2-phenylimidazo[1,2-a]pyridine (2b):** Yield (142 mg, 85%); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.06 (d, J = 7.2 Hz, 2H), 8.01 (s, 1H), 7.55 (d, J = 9.1 Hz, 1H), 7.50-7.46 (m, J = 7.5 Hz, 2H), 7.41-7.37 (m, J = 7.4 Hz, 1H), 7.13 (d, J = 9.1 Hz, 1H), 2.42 (s, 3H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 147.59, 147.06, 133.54, 128.89, 128.50, 128.36, 128.29, 124.33, 123.14, 116.88, 59.11, 18.39. ESI-HRMS (m/z): calcd for C<sub>14</sub>H<sub>12</sub>IN<sub>2</sub> [M + H]<sup>+</sup>, 335.0045; found, 335.0048.



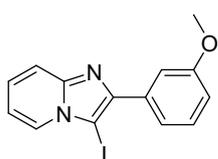
**8-Iodo-5-methyl-2-phenylimidazo[1,2-a]pyridine (2c):** Yield (116 mg, 69%); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.11 (d, *J* = 6.8 Hz, 1H), 8.06 (d, *J* = 7.4 Hz, 2H), 7.50-7.46 (m, 2H), 7.41 (d, *J* = 13.4 Hz, 2H), 6.78 (d, *J* = 7.0 Hz, 1H), 2.46 (s, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 148.43, 147.76, 136.69, 133.71, 128.45, 128.35, 128.23, 125.64, 116.01, 115.77, 58.25, 21.31. ESI-HRMS (*m/z*): calcd for C<sub>14</sub>H<sub>12</sub>IN<sub>2</sub> [M + H]<sup>+</sup>, 335.0045; found, 335.0048.



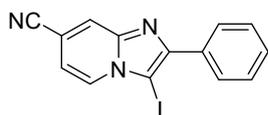
**6-Chloro-3-iodo-2-phenylimidazo[1,2-a]pyridine (2d):** Yield (120 mg, 68%); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.31 (s, 1H), 8.05 (d, *J* = 7.3 Hz, 2H), 7.66 (d, *J* = 9.4 Hz, 1H), 7.52-7.48 (m, 3H), 7.44 (d, *J* = 7.2 Hz, 1H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 148.74, 146.30, 132.82, 128.77, 128.54, 128.50, 128.49, 127.35, 124.66, 121.90, 117.87, 60.41. ESI-HRMS (*m/z*): calcd for C<sub>13</sub>H<sub>9</sub>ClIN<sub>2</sub> [M + H]<sup>+</sup>, 354.9499; found, 354.9503.



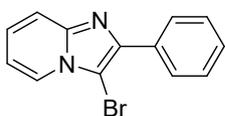
**6-Bromo-3-iodo-2-phenylimidazo[1,2-a]pyridine (2e):** Yield (160 mg, 80%); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.38 (s, 1H), 8.04 (d, *J* = 7.1 Hz, 2H), 7.52 – 7.47 (m, 3H), 7.42 (d, *J* = 7.3 Hz, 1H), 7.33 (dd, *J* = 9.4, 1.8 Hz, 1H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 148.86, 146.66, 133.11, 129.08, 128.64, 128.50, 128.46, 126.76, 118.20, 108.06, 59.87; ESI-HRMS (*m/z*): calcd for C<sub>13</sub>H<sub>9</sub>BrIN<sub>2</sub> [M + H]<sup>+</sup>, 398.8994; found, 398.8998.



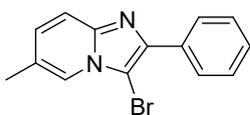
**3-Iodo-2-(3-methoxyphenyl)imidazo[1,2-a]pyridine (2f):** Yield (126 mg, 72%); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.23 (d, *J* = 6.9 Hz, 1H), 7.67 (d, *J* = 7.7 Hz, 1H), 7.62 (d, *J* = 8.7 Hz, 2H), 7.41-7.37 (m, *J* = 7.9 Hz, 1H), 7.27 (d, *J* = 6.8 Hz, 1H), 6.98 – 6.90 (m, 2H), 3.90 (s, 3H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 159.59, 148.02, 147.83, 134.80, 129.42, 126.59, 125.73, 121.05, 117.60, 114.68, 113.53, 113.31, 59.82, 55.42. ESI-HRMS (*m/z*): calcd for C<sub>14</sub>H<sub>12</sub>IN<sub>2</sub>O [M + H]<sup>+</sup>, 350.9994; found, 350.9998.



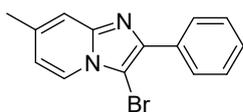
**3-Iodo-2-phenylimidazo[1,2-a]pyridine-7-carbonitrile (2g):** Yield (92 mg, 54%); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.33 (dd, *J* = 7.1, 0.9 Hz, 1H), 8.06 (t, *J* = 1.8 Hz, 1H), 8.05 – 8.04 (m, 1H), 8.01 (dd, *J* = 1.6, 0.9 Hz, 1H), 7.55 – 7.49 (m, 2H), 7.48 – 7.43 (m, 1H), 7.09 (dd, *J* = 7.1, 1.6 Hz, 1H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 151.16, 146.04, 132.48, 129.19, 128.63, 127.36, 123.25, 117.40, 113.48, 108.23, 63.85. ESI-HRMS (*m/z*): calcd for C<sub>14</sub>H<sub>9</sub>IN<sub>3</sub> [M + H]<sup>+</sup>, 345.9841; found, 345.9952.



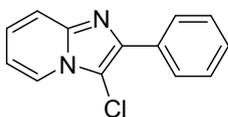
**3-Bromo-2-phenylimidazo[1,2-a]pyridine (2h):** Yield (83 mg, 61%); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.19 (d, *J* = 6.9 Hz, 1H), 8.13 (d, *J* = 7.3 Hz, 2H), 7.65 (d, *J* = 9.1 Hz, 1H), 7.48 (t, *J* = 7.5 Hz, 2H), 7.39 (t, *J* = 7.3 Hz, 1H), 7.25 (d, *J* = 4.4 Hz, 1H), 6.94 (t, *J* = 6.5 Hz, 1H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 145.48, 142.74, 132.77, 128.79, 128.45, 128.31, 127.94, 125.10, 123.97, 117.66, 113.07; ESI-HRMS (*m/z*): calcd for C<sub>13</sub>H<sub>10</sub>BrN<sub>2</sub> [M + H]<sup>+</sup>, 273.0027; found, 273.0029.



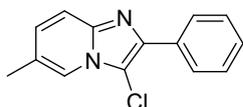
**3-Bromo-6-methyl-2-phenylimidazo[1,2-a]pyridine (2i):** Yield (95 mg, 66%); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.11 (d, *J* = 7.3 Hz, 2H), 7.96 (s, 1H), 7.54 (d, *J* = 9.2 Hz, 1H), 7.47 (t, *J* = 7.6 Hz, 2H), 7.38 (d, *J* = 7.3 Hz, 1H), 7.11 (d, *J* = 9.1 Hz, 1H), 2.40 (s, 3H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 144.43, 142.25, 128.79, 128.50, 128.46, 128.24, 127.85, 127.30, 123.08, 121.71, 116.88, 18.39. ESI-HRMS (*m/z*): calcd for C<sub>14</sub>H<sub>12</sub>BrN<sub>2</sub> [M + H]<sup>+</sup>, 287.0184; found, 287.0182.



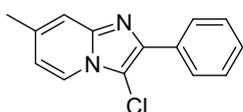
**3-Bromo-7-methyl-2-phenylimidazo[1,2-a]pyridine (2j):** Yield (84 mg, 59%)<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.11 (dd, J = 8.3, 1.2 Hz, 2H), 8.04 (d, J = 7.0 Hz, 1H), 7.47 (t, J = 7.5 Hz, 2H), 7.40 – 7.35 (m, 2H), 6.75 (dd, J = 7.0, 1.5 Hz, 1H), 2.43 (s, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 145.84, 142.32, 136.21, 133.04, 128.45, 128.16, 127.81, 123.15, 116.03, 115.69, 90.83, 21.37. ESI-HRMS (*m/z*): calcd for C<sub>14</sub>H<sub>12</sub>BrN<sub>2</sub> [M + H]<sup>+</sup>, 287.0184; found, 287.0182.



**3-Chloro-2-phenylimidazo[1,2-a]pyridine (2k):** Yield (43 mg, 38%); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.16 – 8.11 (m, 3H), 7.71 (d, J = 9.1 Hz, 1H), 7.49 (t, J = 7.5 Hz, 2H), 7.40 (d, J = 7.4 Hz, 1H), 7.26 (t, J = 7.9 Hz, 1H), 6.95 (t, J = 6.8 Hz, 1H). <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 143.71, 139.70, 133.01, 128.59, 128.35, 127.60, 125.11, 122.71, 117.62, 113.09, 105.82; ESI-HRMS (*m/z*): calcd for C<sub>13</sub>H<sub>10</sub>ClN<sub>2</sub> [M + H]<sup>+</sup>, 229.0533; found, 229.0536.

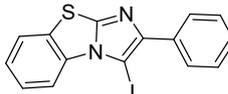


**3-Chloro-6-methyl-2-phenylimidazo[1,2-a]pyridine (2l):** Yield (56 mg, 46%); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.12 (dd, J = 8.3, 1.2 Hz, 2H), 7.84 (s, 1H), 7.53 – 7.44 (m, 3H), 7.36 (t, J = 7.4 Hz, 1H), 7.05 (d, J = 9.2 Hz, 1H), 2.34 (s, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 142.79, 139.47, 132.71, 128.53, 128.10, 128.07, 127.79, 127.37, 122.77, 120.33, 116.91, 105.26, 18.38. ESI-HRMS (*m/z*): calcd for C<sub>14</sub>H<sub>12</sub>ClN<sub>2</sub> [M + H]<sup>+</sup>, 243.0689; found, 243.0692.

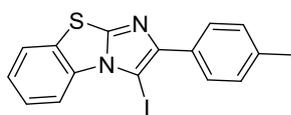


**3-Chloro-7-methyl-2-phenylimidazo[1,2-a]pyridine (2m):** Yield (59 mg, 49%); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.12 (d, J = 7.2 Hz, 2H), 7.99 (d, J = 7.0 Hz, 1H), 7.48 (t, J = 7.8 Hz, 2H), 7.38 (dd, J = 13.3, 6.0 Hz, 2H), 6.77 (d, J = 7.0 Hz, 1H), 2.43 (s, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 144.12, 139.34, 136.09, 132.62, 128.54, 128.13, 127.43, 121.91, 116.01, 115.62, 105.04, 21.42; ESI-HRMS (*m/z*): calcd for C<sub>14</sub>H<sub>12</sub>ClN<sub>2</sub> [M + H]<sup>+</sup>, 243.0689; found, 243.0695.

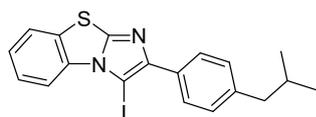
### 3.2. Typical procedure for the synthesis of 3-iodo-2-phenylbenzo[d]imidazo[2,1-b]thiazole (6a):



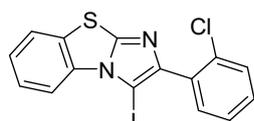
2-phenylbenzo[d]imidazo[2,1-b]thiazole-3-carbaldehyde **5a** (127 mg, 0.5 mmol) dissolved in acetonitrile (3 mL) was mixed with aq. TBHP (70 % in water, 192 μL, 1.5 mmol) and molecular iodine (127 mg, 0.5 mmol). The reaction was stirred at 60°C for 6h and monitored by TLC for completion. The mixture was cooled to rt, quenched with saturated sodium thiosulfate and extracted with EtOAc (10×3 ml). The combined organic layer was dried over Na<sub>2</sub>SO<sub>4</sub>, concentrated using rotary evaporator and purified by column chromatography on silica gel using n-hexane/ethyl acetate (1:9) as an eluent to obtain compound **6a** as white solid (128 mg, 68 % yield). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.26 (d, J = 8.2 Hz, 1H), 8.04 (dd, J = 8.2, 1.0 Hz, 2H), 7.70 (d, J = 8.0 Hz, 1H), 7.48-7.44 (m, 3H), 7.40 – 7.34 (m, 2H). <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 146.19 (C), 141.27 (C), 132.63 (C), 132.53 (C), 130.10 (C), 128.53 (CH), 127.80 (CH), 126.71 (CH), 126.13 (CH), 125.20 (CH), 124.23 (CH), 113.53 (CH), 108.46 (C). ESI-HRMS (*m/z*): calcd for C<sub>15</sub>H<sub>10</sub>IN<sub>2</sub>S [M + H]<sup>+</sup>, 376.9609; found, 376.9613.



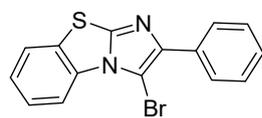
**3-Iodo-2-(p-tolyl)benzo[d]imidazo[2,1-b]thiazole (6b):** Yield (142 mg, 73%); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.65 (d, J = 8.2 Hz, 1H), 7.81 (d, J = 7.9 Hz, 2H), 7.67 (d, J = 7.9 Hz, 1H), 7.43 (t, J = 7.8 Hz, 1H), 7.36 (t, J = 7.6 Hz, 1H), 7.22 (s, 2H), 2.37 (s, 3H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 150.62, 137.95, 133.80, 130.60, 130.52, 129.83, 129.05, 128.02, 127.55, 125.46, 125.24, 124.31, 113.89, 53.77, 21.39. ESI-HRMS (*m/z*): calcd for C<sub>16</sub>H<sub>12</sub>IN<sub>2</sub>S [M + H]<sup>+</sup>, 390.9766; found, 390.9774.



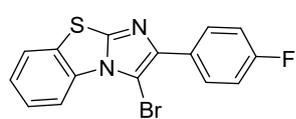
**3-Iodo-2-(4-isobutylphenyl)benzo[d]imidazo[2,1-b]thiazole (6c):** Yield (150 mg, 70%);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.73 (d,  $J = 8.2$  Hz, 1H), 7.90 (d,  $J = 7.9$  Hz, 2H), 7.74 (d,  $J = 8.0$  Hz, 1H), 7.53-7.49 (m, 1H), 7.45-7.41 (m, 1H), 7.28 (d,  $J = 3.8$  Hz, 2H), 2.56 (d,  $J = 7.1$  Hz, 2H), 1.95 (dt,  $J = 13.4, 6.7$  Hz, 1H), 0.97 (d,  $J = 6.6$  Hz, 6H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  150.98, 150.45, 141.75, 133.81, 130.83, 130.51, 129.10, 127.81, 125.44, 125.22, 124.30, 113.89, 53.88, 45.30, 30.26, 22.45. ESI-HRMS ( $m/z$ ): calcd for  $\text{C}_{19}\text{H}_{18}\text{IN}_2\text{S}$  [ $\text{M}^+ \text{H}$ ] $^+$ , 433.0235; found, 433.0238.



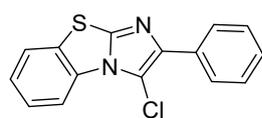
**2-(2-Chlorophenyl)-3-iodobenzo[d]imidazo[2,1-b]thiazole (6d):**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.62 (d,  $J = 8.2$  Hz, 1H), 7.74 (d,  $J = 7.9$  Hz, 1H), 7.50 (dd,  $J = 11.1, 7.0$  Hz, 3H), 7.43 (d,  $J = 7.8$  Hz, 1H), 7.39 – 7.34 (m, 2H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3 + \text{CH}_3\text{OD}$ )  $\delta$  150.49, 149.05, 134.18, 133.31, 132.54, 132.26, 132.02, 130.30, 130.24, 129.84, 126.62, 125.71, 124.38, 113.87, 59.35; LCMS (ESI-TOF):  $m/z$ : [ $\text{M}^+ \text{H}$ ] $^+$  calcd for  $\text{C}_{15}\text{H}_9\text{ClIN}_2\text{S}$ , 410.92; found, 411.10.



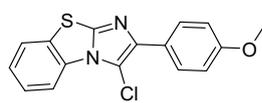
**3-Bromo-2-phenylbenzo[d]imidazo[2,1-b]thiazole (6e):** Yield (92 mg, 53%);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.43 (d,  $J = 8.1$  Hz, 1H), 8.03 (d,  $J = 7.3$  Hz, 2H), 7.70 (d,  $J = 7.8$  Hz, 1H), 7.46 (t,  $J = 7.4$  Hz, 3H), 7.37 (d,  $J = 6.8$  Hz, 2H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  148.14, 144.40, 132.84, 130.26, 128.43, 127.93, 127.28, 125.90, 125.23, 124.24, 113.73, 113.52, 91.88; ESI-HRMS ( $m/z$ ): calcd for  $\text{C}_{15}\text{H}_{10}\text{BrN}_2\text{S}$  [ $\text{M}^+ \text{H}$ ] $^+$ , 328.9748; found, 328.9747.



**3-Bromo-2-(4-fluorophenyl)benzo[d]imidazo[2,1-b]thiazole (6f):** Yield (81 mg, 49%);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.43 (d,  $J = 8.1$  Hz, 1H), 8.00 (s, 2H), 7.71 (d,  $J = 7.8$  Hz, 1H), 7.47 (t,  $J = 7.8$  Hz, 1H), 7.40 (d,  $J = 7.5$  Hz, 1H), 7.14 (t,  $J = 8.3$  Hz, 2H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  133.08 (s), 130.25 (s), 129.13 (d,  $J = 8.4$  Hz), 128.58 (d,  $J = 8.0$  Hz), 126.18 (s), 125.95 (s), 125.32 (s), 125.27 (s), 124.27 (s), 115.53 (d,  $J = 9.4$  Hz), 115.31 (d,  $J = 9.3$  Hz), 113.70 (s), 113.50 (s); found, 346.9660.

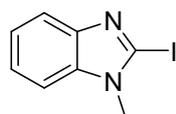


**3-Chloro-2-phenylbenzo[d]imidazo[2,1-b]thiazole (6g):** Yield (49 mg, 35%);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.24 (d,  $J = 8.2$  Hz, 1H), 8.05 – 8.01 (m, 2H), 7.69 (d,  $J = 8.0$  Hz, 1H), 7.49 – 7.42 (m, 3H), 7.39 – 7.32 (m, 2H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  146.13, 141.20, 132.55, 132.49, 130.03, 128.50, 127.76, 126.66, 126.08, 125.14, 124.17, 113.46, 108.42; ESI-HRMS ( $m/z$ ): calcd for  $\text{C}_{15}\text{H}_{10}\text{ClN}_2\text{S}$  [ $\text{M}^+ \text{H}$ ] $^+$ , 285.0253; found, 285.0262.

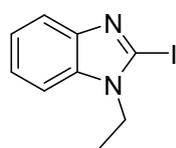


**3-Chloro-2-(4-methoxyphenyl)benzo[d]imidazo[2,1-b]thiazole (6h):** Yield (65 mg, 42%);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.21 (d,  $J = 8.2$  Hz, 1H), 7.97 – 7.93 (m, 2H), 7.67 (d,  $J = 7.9$  Hz, 1H), 7.45 – 7.40 (m, 1H), 7.36 – 7.31 (m, 1H), 7.01 – 6.97 (m, 2H), 3.85 (s, 3H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  159.24, 145.94, 141.17, 132.69, 132.63, 129.97, 128.54, 128.02, 126.07, 125.01, 124.17, 113.93, 113.36, 107.42, 55.33; ESI-HRMS ( $m/z$ ): calcd for  $\text{C}_{16}\text{H}_{12}\text{ClN}_2\text{OS}$  [ $\text{M}^+ \text{H}$ ] $^+$ , 315.0359; found, 315.0367.

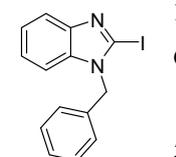
### 3.3. Typical procedure for the 2-iodo-1-methyl-1H-benzo[d]imidazole (8a):



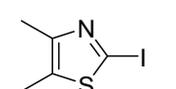
A mixture of 1-methyl-1H-benzo[d]imidazole-2-carbaldehyde **7a** (80 mg, 0.5 mmol), TBHP (70 % in water, 192 $\mu$ L, 1.5 mmol) and molecular iodine (127 mg, 0.5 mmol) in acetonitrile (3 mL) was refluxed at 90°C for 5h and reaction progress was monitored by TLC. The reaction mixture was cooled to room temperature and unreacted iodine was quenched with saturated sodium thiosulphate solution. The resulting mixture was extracted with EtOAc (10 $\times$ 3 ml), dried over Na<sub>2</sub>SO<sub>4</sub> and concentrated using rotary evaporator. The residue was purified by column chromatography on silica gel using n-hexane/ethyl acetate as an eluent to obtain **8a** as yellow solid (70 mg, 54%yield); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.74 – 7.70 (m, 1H), 7.35 – 7.32 (m, 1H), 7.25 – 7.19 (m, 2H), 3.77 (s, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  145.45 (C), 136.33 (C), 123.08 (CH), 122.27 (CH), 119.24 (CH), 109.37 (CH), 104.27 (C), 33.73 (CH<sub>3</sub>). ESI-HRMS (*m/z*): calcd for C<sub>8</sub>H<sub>8</sub>IN<sub>2</sub> [M+ H]<sup>+</sup>, 258.9732; found, 258.9729.



**1-Ethyl-2-iodo-1H-benzo[d]imidazole (8b):** Yield (78 mg, 57%); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.80 – 7.73 (m, 1H), 7.39 (d, J = 6.9 Hz, 1H), 7.31 – 7.24 (m, 2H), 4.26 (q, J = 7.2 Hz, 2H), 1.43 (s, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  145.81, 135.25, 123.00, 122.22, 119.37, 109.30, 102.83, 42.26, 14.87; ESI-HRMS (*m/z*): calcd for C<sub>9</sub>H<sub>10</sub>IN<sub>2</sub> [M+ H]<sup>+</sup>, 272.9889; found, 272.9896.

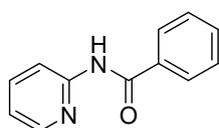


**1-Benzyl-2-iodo-1H-benzo[d]imidazole (8c):** Yield (114 mg, 68%); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.75 (d, J = 7.6 Hz, 1H), 7.30 (d, J = 7.5 Hz, 2H), 7.23 (d, J = 2.2 Hz, 1H), 7.21 (d, J = 1.3 Hz, 1H), 7.19 (dd, J = 3.5, 1.5 Hz, 1H), 7.16 (d, J = 1.0 Hz, 1H), 7.13 (d, J = 6.2 Hz, 2H), 5.37 (s, 2H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>)  $\delta$  145.73, 135.81, 135.15, 128.99, 128.14, 126.73, 123.33, 122.52, 119.35, 109.98, 104.20, 50.66 . ESI-HRMS (*m/z*): calcd for C<sub>14</sub>H<sub>12</sub>IN<sub>2</sub> [M+ H]<sup>+</sup>, 335.0045; found, 335.0054.

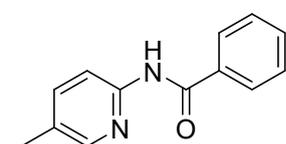


**2-Iodo-4,5-dimethylthiazole (8e):** Yield (66 mg, 56%); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  2.34 (s, 6H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  151.01, 132.85, 94.87, 14.52 , 11.07 ; LCMS (ESI-TOF): *m/z*: [M+H]<sup>+</sup> calcd for C<sub>5</sub>H<sub>7</sub>INS, 239.93; found, 239.98.

### Typical procedure for the synthesis of N-(pyridin-2-yl)benzamide (3a)

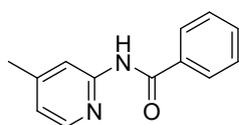


To a 25 mL round bottom flask was added 2-phenylimidazo[1,2-*a*]pyridine-3-carbaldehyde **1a** (111 mg, 0.5 mmol), acetonitrile (3 mL) and TBHP (70 % in water, 192 $\mu$ L, 1.5 mmol). The reaction mixture was then stirred under air atmosphere at 80°C for 15 h. The reaction progress was monitored by TLC and was allowed to cool down after completion. The solvent was removed under reduced pressure and residue was purified by column chromatography on silica gel using petroleum ether/ethyl acetate as an eluent to provide the desired product **3a** (74 mg, 75% yield) . <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.78 (s, 1H), 8.41 (d, J = 8.4 Hz, 1H), 8.28 (dd, J = 4.9, 1.0 Hz, 1H), 7.94 (d, J = 7.1 Hz, 2H), 7.80 – 7.74 (m, 1H), 7.58 (t, J = 7.3 Hz, 1H), 7.51 (t, J = 7.4 Hz, 2H), 7.08 (ddd, J = 7.3, 4.9, 1.0 Hz, 1H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>)  $\delta$  166.02, 151.70, 147.47, 138.80, 134.22, 132.27, 128.79, 127.43, 119.92, 114.56. ESI-HRMS (*m/z*): calcd for C<sub>12</sub>H<sub>11</sub>N<sub>2</sub>O [M+ H]<sup>+</sup>, 199.0871; found, 199.0873.

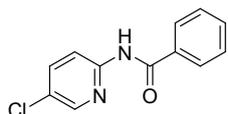


**N-(5-Methylpyridin-2-yl)benzamide (3b):** Yield (76 mg, 71%); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  9.23 (s, 1H), 8.34 (d, J = 8.6 Hz, 1H), 8.11 (d, J = 2.3 Hz, 1H), 8.00 (d, J = 1.2 Hz, 1H), 7.98 (d, J = 1.5 Hz, 1H), 7.59 (dd, J = 11.3, 6.4, 2.6, 1.0

Hz, 2H), 7.51 (ddd,  $J = 8.3, 2.5, 1.0$  Hz, 2H), 2.33 (s, 3H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  165.91, 149.48, 147.12, 139.50, 132.18, 129.95, 128.35, 127.42, 114.16, 17.73. ESI-HRMS ( $m/z$ ): calcd for  $\text{C}_{13}\text{H}_{13}\text{N}_2\text{O}$  [ $\text{M} + \text{H}$ ] $^+$ , 213.1028; found, 213.1031.

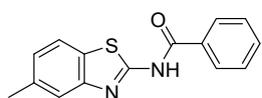


**N-(4-Methylpyridin-2-yl)benzamide (3c):** Yield (72 mg, 68%);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.80 (s, 1H), 8.26 (s, 1H), 8.12 (d,  $J = 5.1$  Hz, 1H), 7.94 (d,  $J = 7.3$  Hz, 2H), 7.57 (t,  $J = 7.3$  Hz, 1H), 7.50 (t,  $J = 7.5$  Hz, 2H), 6.90 (d,  $J = 5.0$  Hz, 1H), 2.41 (s, 3H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  151.57, 150.27, 147.25, 134.30, 132.24, 129.91, 128.83, 128.32, 127.28, 121.17, 114.82, 21.51; ESI-HRMS ( $m/z$ ): calcd for  $\text{C}_{13}\text{H}_{13}\text{N}_2\text{O}$  [ $\text{M} + \text{H}$ ] $^+$ , 213.1028; found, 213.1031.

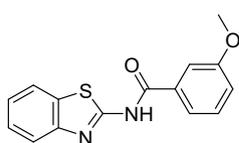


**N-(5-Chloropyridin-2-yl)benzamide (3d):** Yield (69 mg, 60%);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.62 (s, 1H), 8.39 (d,  $J = 8.9$  Hz, 1H), 8.24 (d,  $J = 2.3$  Hz, 1H), 7.92 (d,  $J = 7.4$  Hz, 2H), 7.72 (dd,  $J = 8.9, 2.5$  Hz, 1H), 7.58 (d,  $J = 7.3$  Hz, 1H), 7.53-7.49 (m, 2H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  166.96, 151.32, 147.97, 139.50, 135.37, 133.85, 130.33, 128.61, 128.36, 116.23; ESI-HRMS ( $m/z$ ): calcd for  $\text{C}_{12}\text{H}_{10}\text{ClN}_2\text{O}$  [ $\text{M} + \text{H}$ ] $^+$ , 233.0482; found, 233.0483.

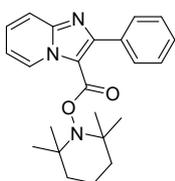
**N-(Benzo[d]thiazol-2-yl)benzamide (3e):** Yield (89 mg, 70%);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.00 (d,  $J = 7.8$  Hz, 2H), 7.87 – 7.82 (m, 1H), 7.56 (t,  $J = 7.4$  Hz, 1H), 7.42 (t,  $J = 7.7$  Hz, 2H), 7.35 – 7.25 (m, 3H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  166.01, 159.80, 147.74, 133.10, 132.01, 131.88, 129.03, 127.98, 126.12, 124.02, 121.40, 120.65. ESI-HRMS ( $m/z$ ): calcd for  $\text{C}_{14}\text{H}_{11}\text{N}_2\text{OS}$  [ $\text{M} + \text{H}$ ] $^+$ , 255.0592; found, 255.0599.



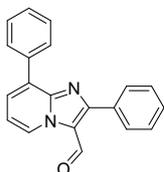
**N-(5-Methylbenzo[d]thiazol-2-yl)benzamide (3f):** Yield (79 mg, 59%);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.93 (s, 1H), 8.31 (d,  $J = 8.5$  Hz, 1H), 8.10 (d,  $J = 7.2$  Hz, 1H), 7.95 (d,  $J = 7.3$  Hz, 2H), 7.61 – 7.54 (m, 2H), 7.51-7.47 (m, 2H), 2.32 (s, 3H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  165.90, 149.39, 146.80, 139.74, 134.20, 132.22, 129.40, 128.77, 127.44, 114.23, 17.87. LCMS (ESI-TOF):  $m/z$ : [ $\text{M} + \text{H}$ ] $^+$  calcd for  $\text{C}_{15}\text{H}_{12}\text{N}_2\text{OS}$ , 268.07; found, 268.13.



**N-(Benzo[d]thiazol-2-yl)-3-methoxybenzamide (3g):** Yield (88 mg, 62%);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.97 (d,  $J = 8.8$  Hz, 2H), 7.86 – 7.82 (m, 1H), 7.34 (dd,  $J = 8.2, 4.9$  Hz, 1H), 7.28 (dt,  $J = 8.9, 3.3$  Hz, 2H), 6.87 (d,  $J = 8.8$  Hz, 2H), 3.81 (s, 3H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  165.49, 163.47, 160.26, 147.70, 131.86, 130.12, 126.05, 124.10, 123.90, 121.38, 120.61, 114.23, 55.55. ESI-HRMS ( $m/z$ ): calcd for  $\text{C}_{16}\text{H}_{15}\text{N}_2\text{O}_2\text{S}$  [ $\text{M} + \text{H}$ ] $^+$ , 285.0698; found, 285.0705.

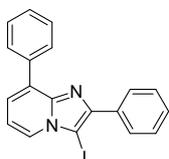


**2,2,6,6-Tetramethylpiperidin-1-yl 2-phenylimidazo[1,2-a]pyridine-3-carboxylate (9):**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  9.55 (dt,  $J = 7.0, 1.1$  Hz, 1H), 7.74 (dt,  $J = 9.0, 1.1$  Hz, 1H), 7.68 – 7.62 (m, 2H), 7.45 (dtd,  $J = 8.6, 7.0, 3.4$  Hz, 4H), 7.07 (td,  $J = 7.0, 1.3$  Hz, 1H), 1.69 (dd,  $J = 20.3, 9.7$  Hz, 2H), 1.59 – 1.34 (m, 4H), 1.05 (s, 6H), 0.74 (s, 6H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  162.17, 153.39, 147.45, 135.41, 129.86, 128.79, 128.59, 128.20, 127.98, 117.43, 114.28, 111.02, 60.22, 39.20, 31.85, 21.01, 16.92; ESI-HRMS ( $m/z$ ): calcd for  $\text{C}_{23}\text{H}_{28}\text{N}_3\text{O}_2$  [ $\text{M} + \text{H}$ ] $^+$ , 378.2182; found, 378.2184.

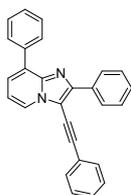


**3-Iodo-2,8-diphenylimidazo[1,2-a]pyridine (10):** Yield (108 mg, 73%);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  10.14 (s, 1H), 9.76 (d,  $J = 6.3$  Hz, 1H), 8.32 (dd,  $J = 36.7, 8.4$  Hz, 5H),

7.85 (d,  $J = 3.5$  Hz, 2H), 7.77 (d,  $J = 7.0$  Hz, 1H), 7.53 (s, 3H), 7.26 (t,  $J = 6.7$  Hz, 1H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  179.86, 158.42, 147.85, 145.81, 141.88, 132.24, 130.11, 130.05, 129.99, 129.26, 128.94, 127.86, 125.04, 123.79, 121.05, 115.35; ESI-HRMS ( $m/z$ ): calcd for  $\text{C}_{20}\text{H}_{15}\text{N}_2\text{O}$   $[\text{M}+\text{H}]^+$ , 299.1184; found, 299.1190.

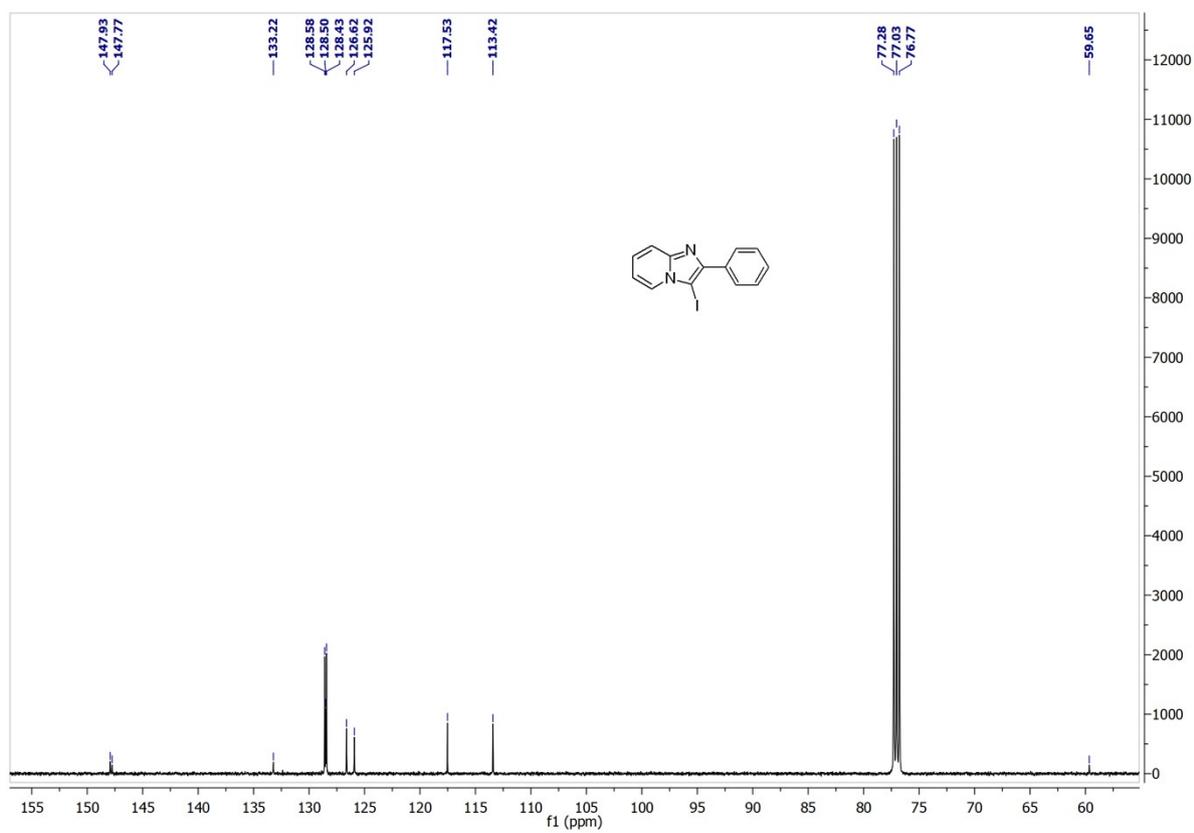
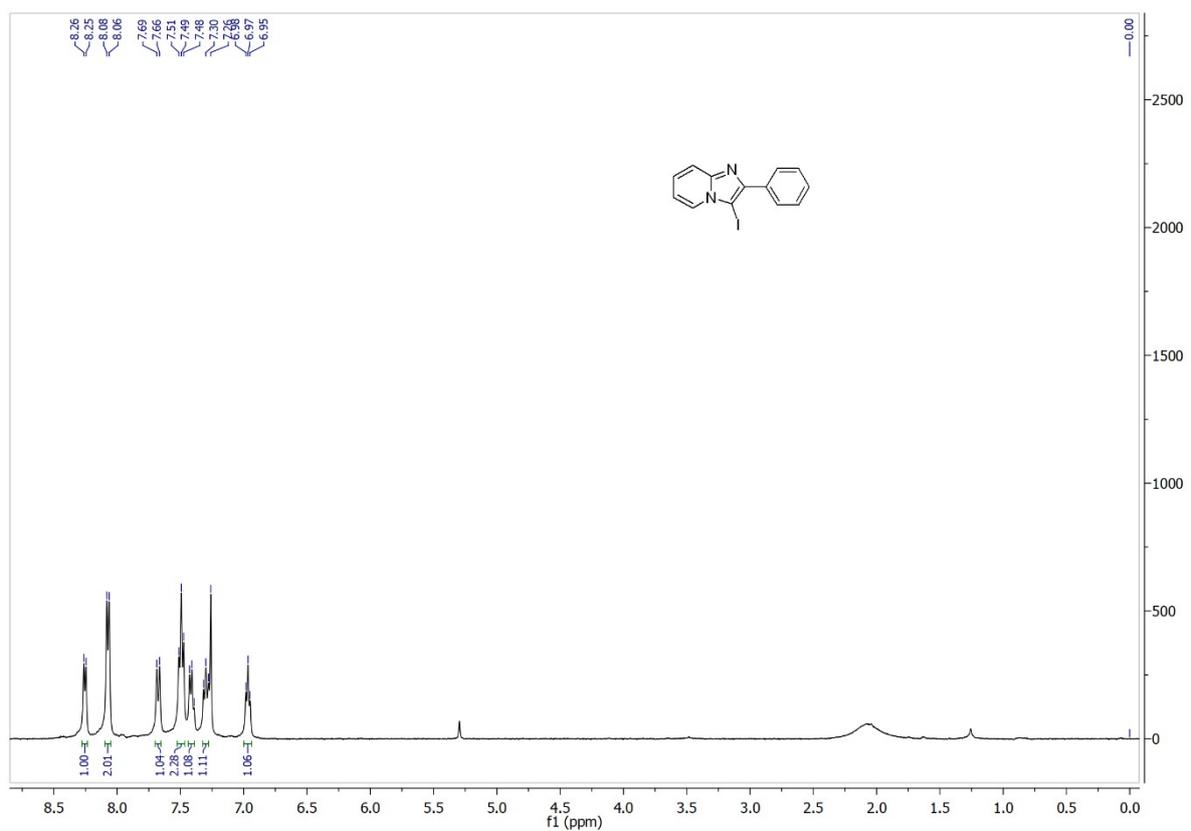


**3-Iodo-2,8-diphenylimidazo[1,2-*a*]pyridine (11):** Yield (88 mg, 67%);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.25 (dd,  $J = 6.8, 1.0$  Hz, 1H), 8.15 – 8.08 (m, 4H), 7.50 (dt,  $J = 12.3, 7.5$  Hz, 4H), 7.44 (d,  $J = 7.3$  Hz, 1H), 7.41 (dd,  $J = 7.2, 0.9$  Hz, 2H), 7.02 (t,  $J = 7.0$  Hz, 1H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  148.04, 146.78, 135.77, 133.73, 130.25, 129.12, 128.64, 128.49, 128.45, 128.26, 128.24, 125.53, 123.87, 113.20, 60.03. ESI-HRMS ( $m/z$ ): calcd for  $\text{C}_{19}\text{H}_{14}\text{N}_2\text{I}$   $[\text{M}+\text{H}]^+$ , 397.0202; found, 397.0209.

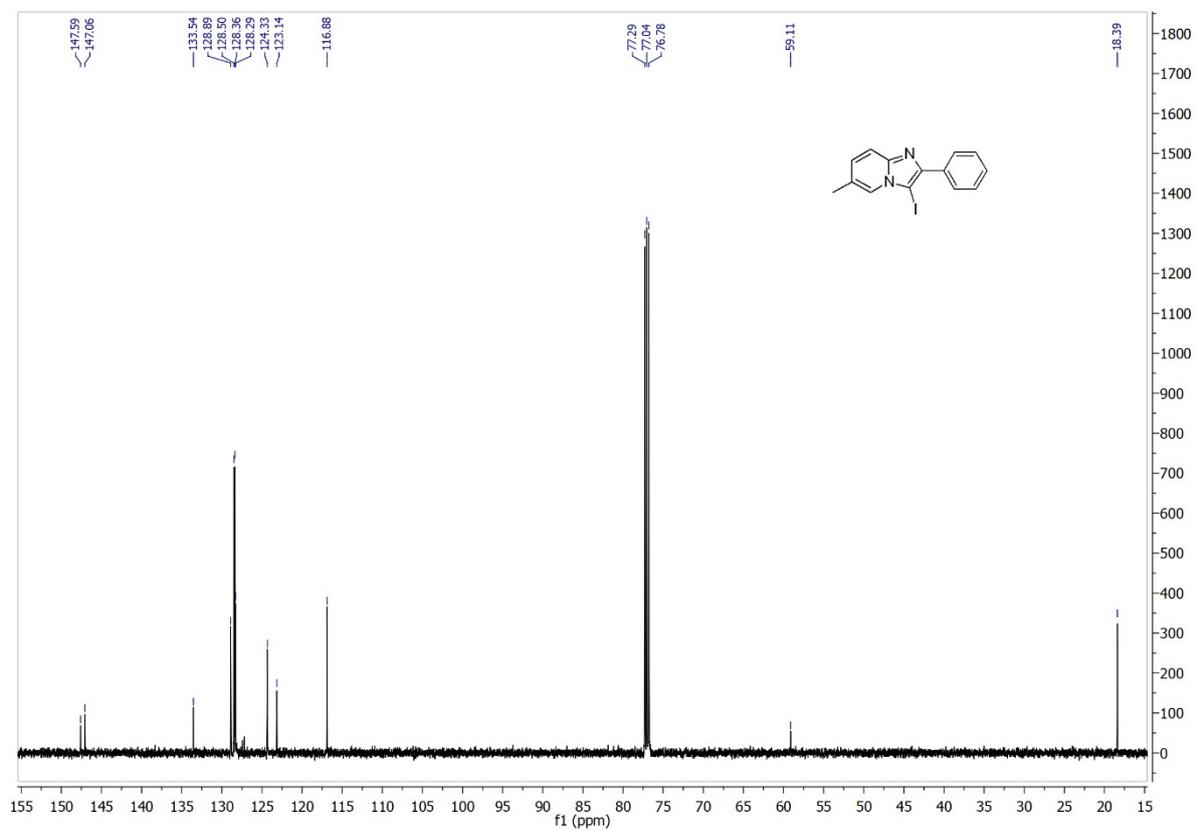
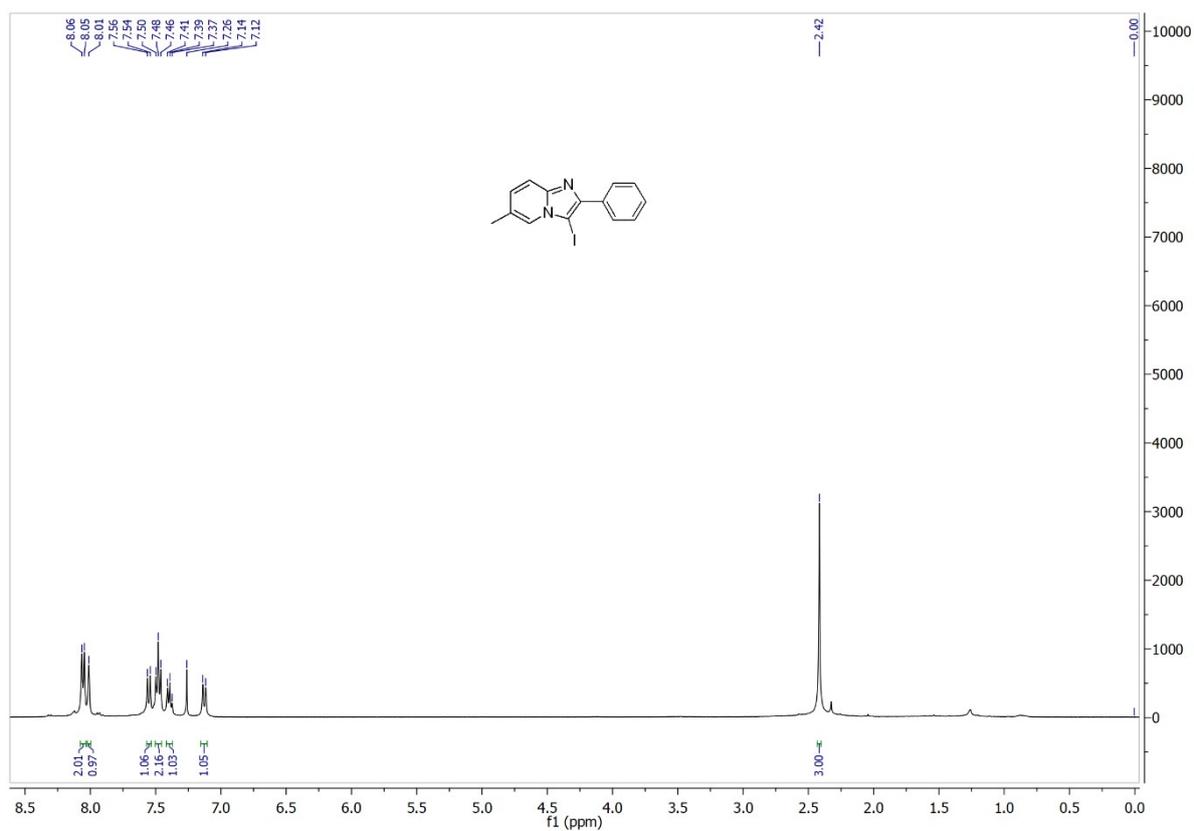


**2,8-Diphenyl-3-(phenylethynyl)imidazo[1,2-*a*]pyridine (12):** Yield (35 mg, 76%);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.44 (d,  $J = 7.3$  Hz, 2H), 8.36 (d,  $J = 6.7$  Hz, 1H), 8.18 – 8.13 (m, 2H), 7.62 (dd,  $J = 7.7, 1.7$  Hz, 2H), 7.56 – 7.45 (m, 5H), 7.41 (ddd,  $J = 8.7, 6.2, 1.9$  Hz, 5H), 7.00 (t,  $J = 6.9$  Hz, 1H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  148.00, 143.94, 136.05, 133.71, 131.28, 130.18, 129.14, 128.72, 128.63, 128.53, 128.49, 127.45, 124.56, 124.11, 122.85, 113.18, 104.99, 101.40, 78.65. ESI-HRMS ( $m/z$ ): calcd for  $\text{C}_{27}\text{H}_{19}\text{N}_2$   $[\text{M}+\text{H}]^+$ , 371.1548; found, 371.1575.

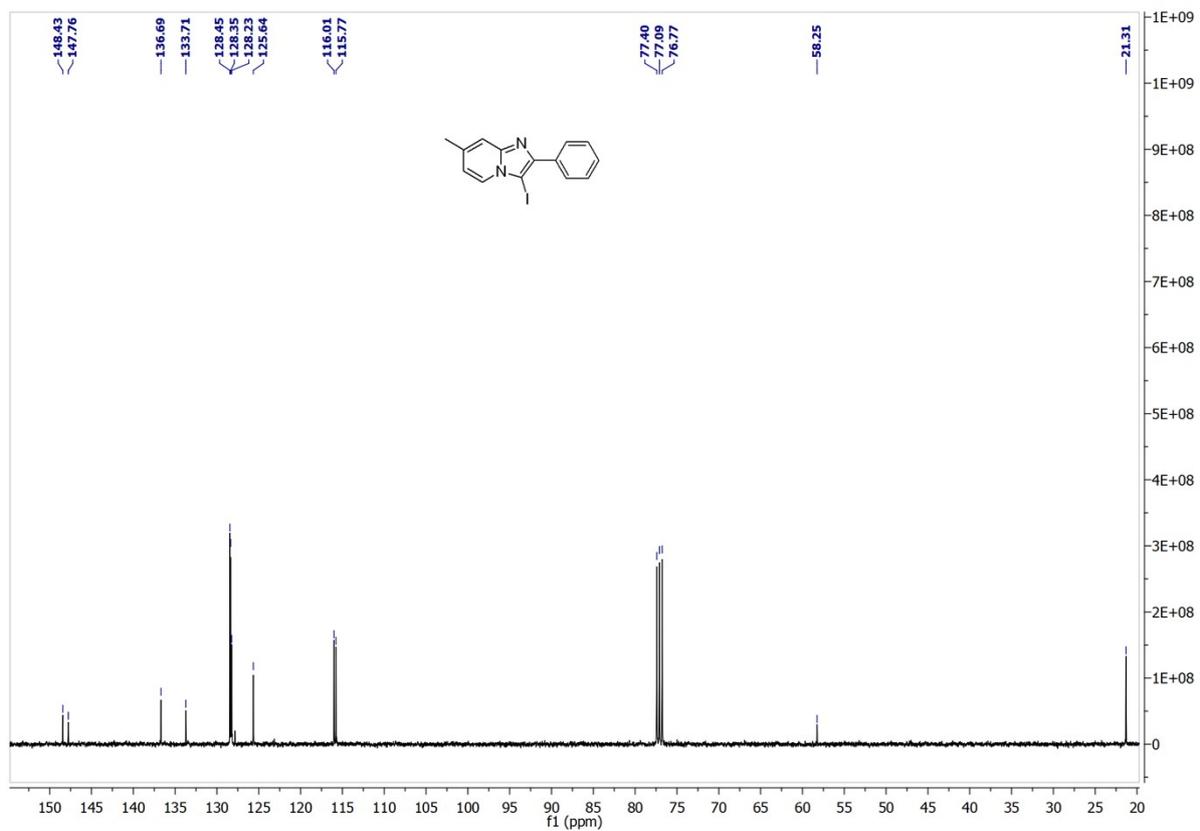
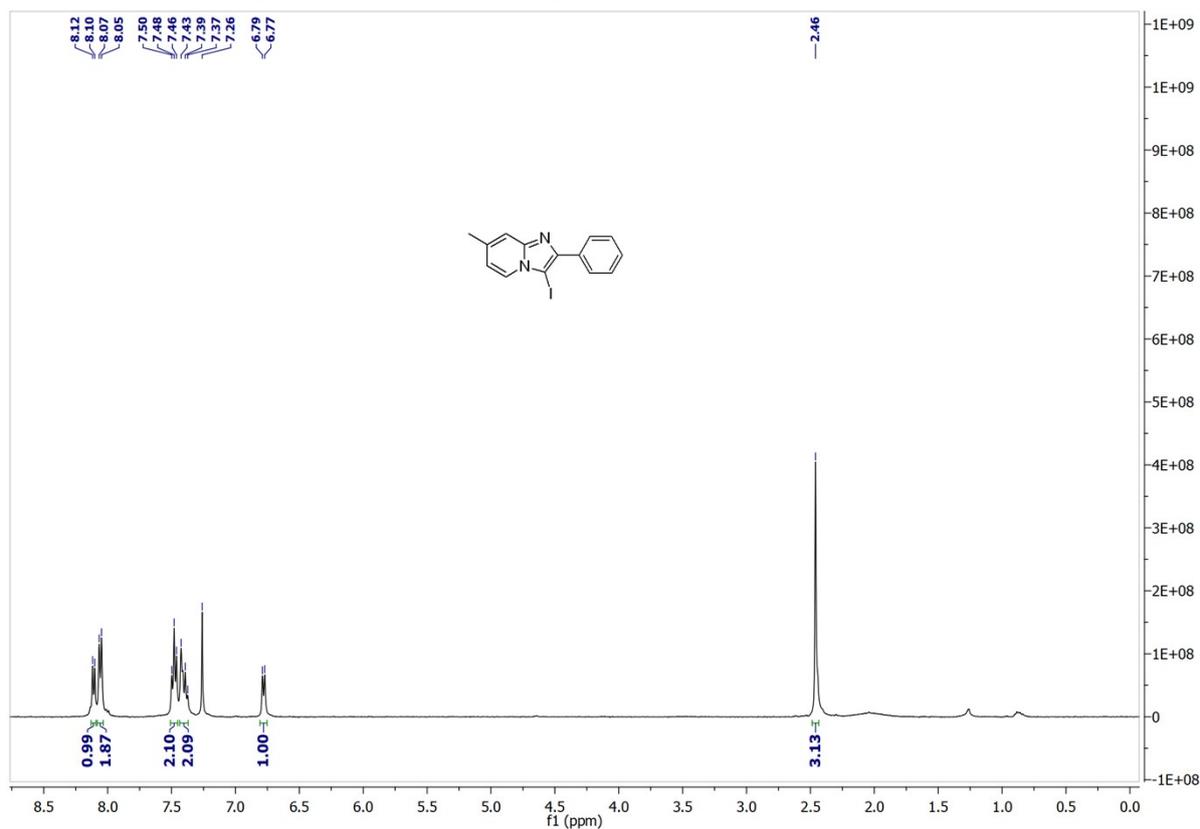
### 3-Iodo-2-phenylimidazo[1,2-a]pyridine (2a)



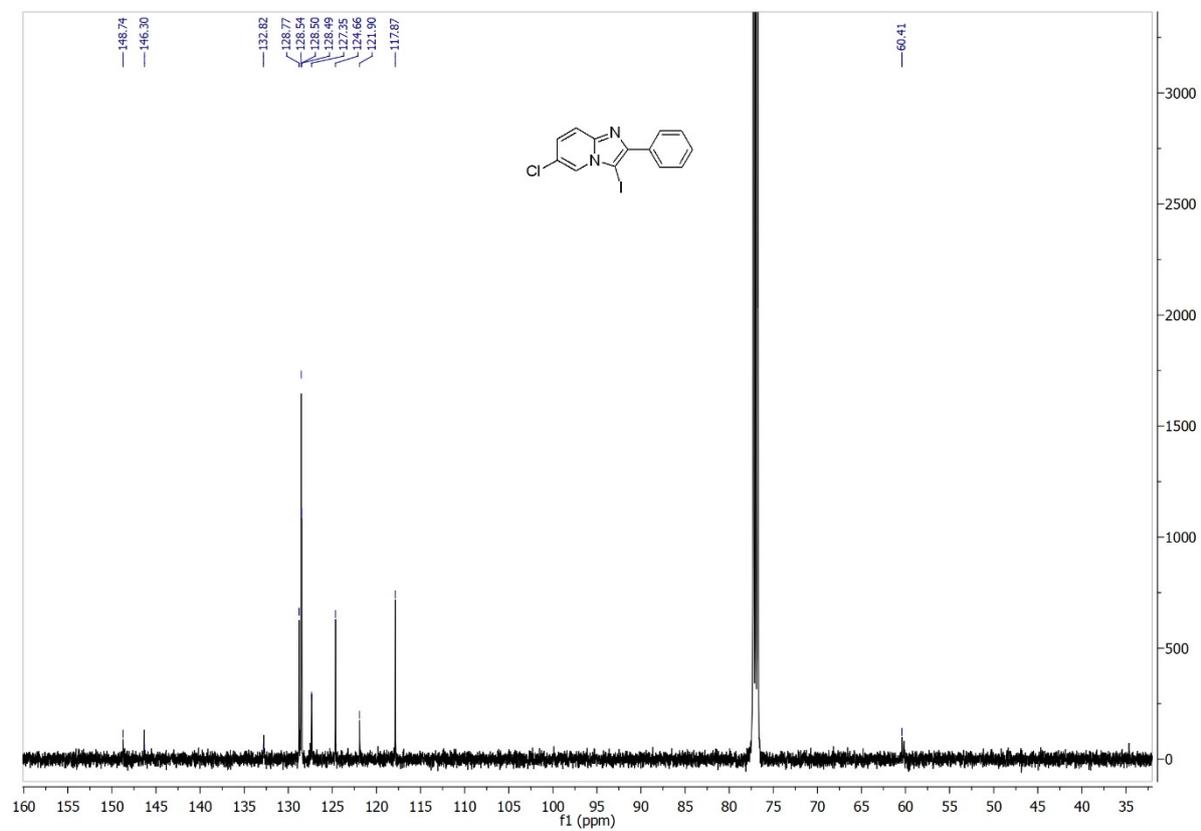
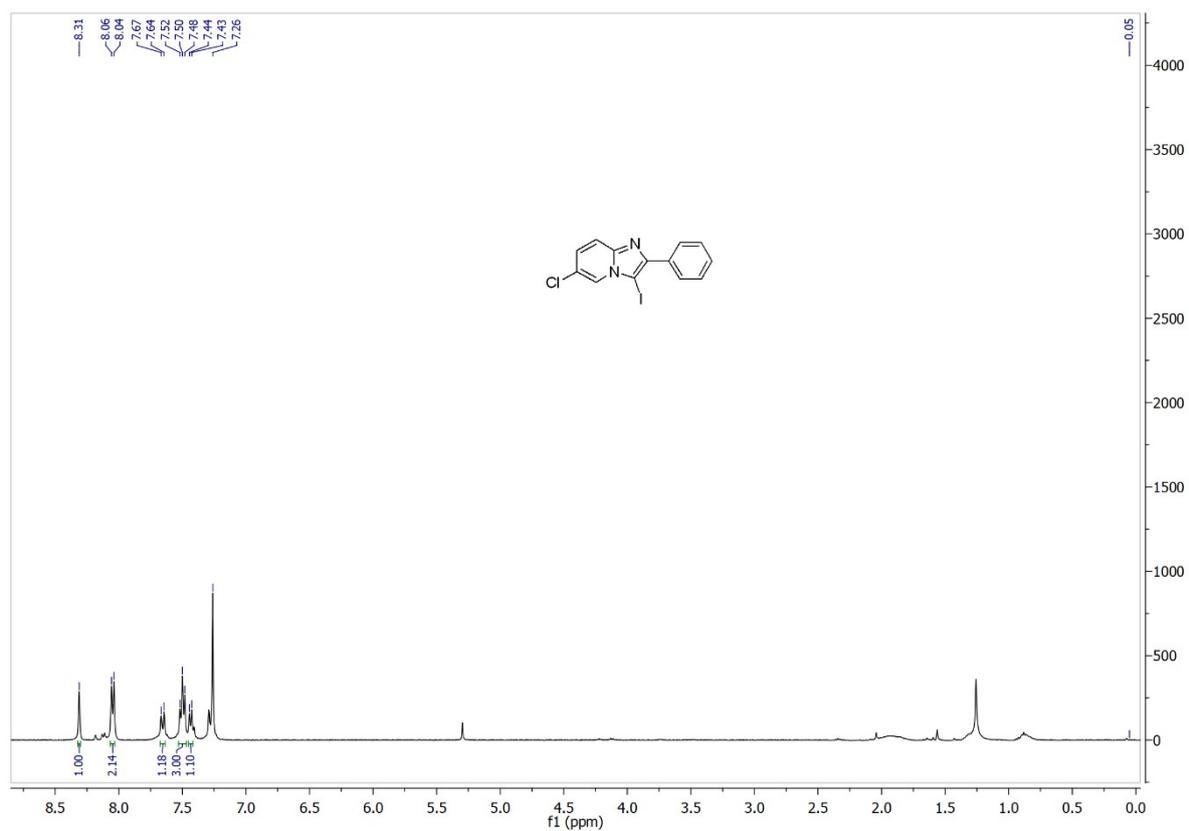
### 3-Iodo-6-methyl-2-phenylimidazo[1,2-a]pyridine (2b)



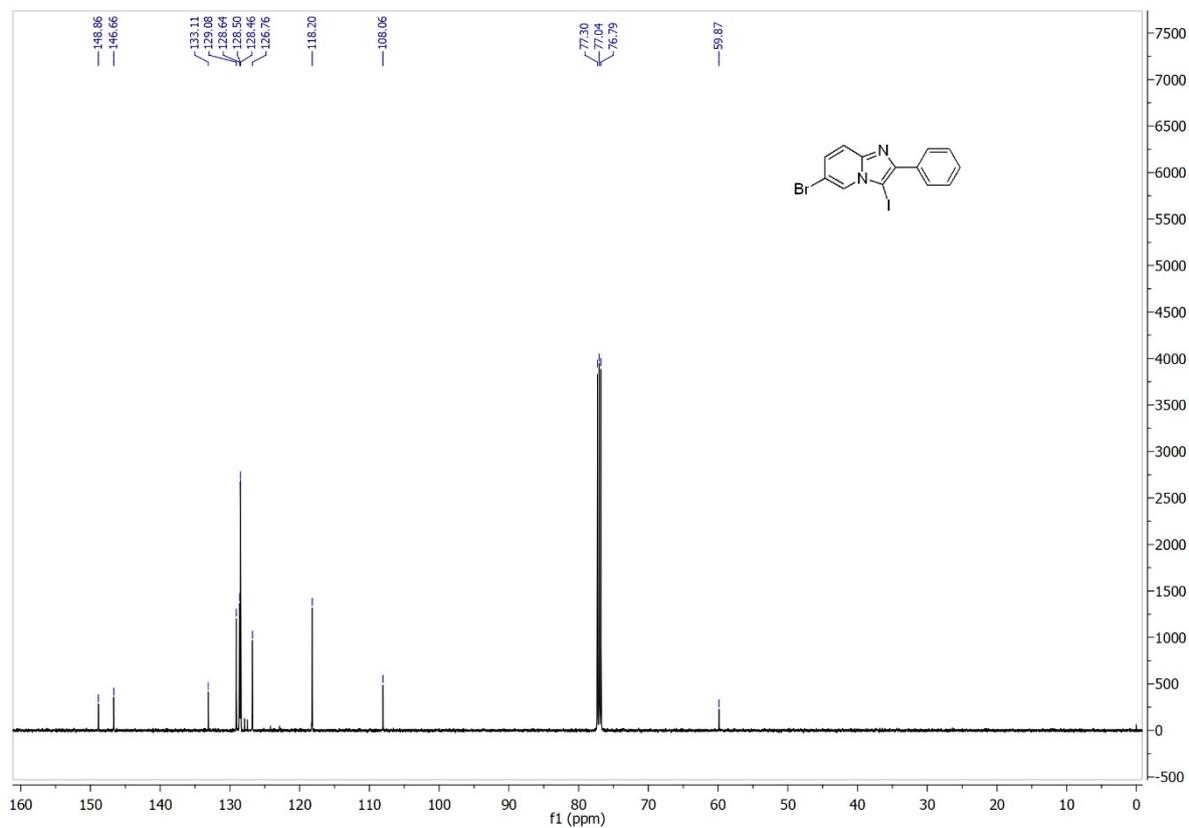
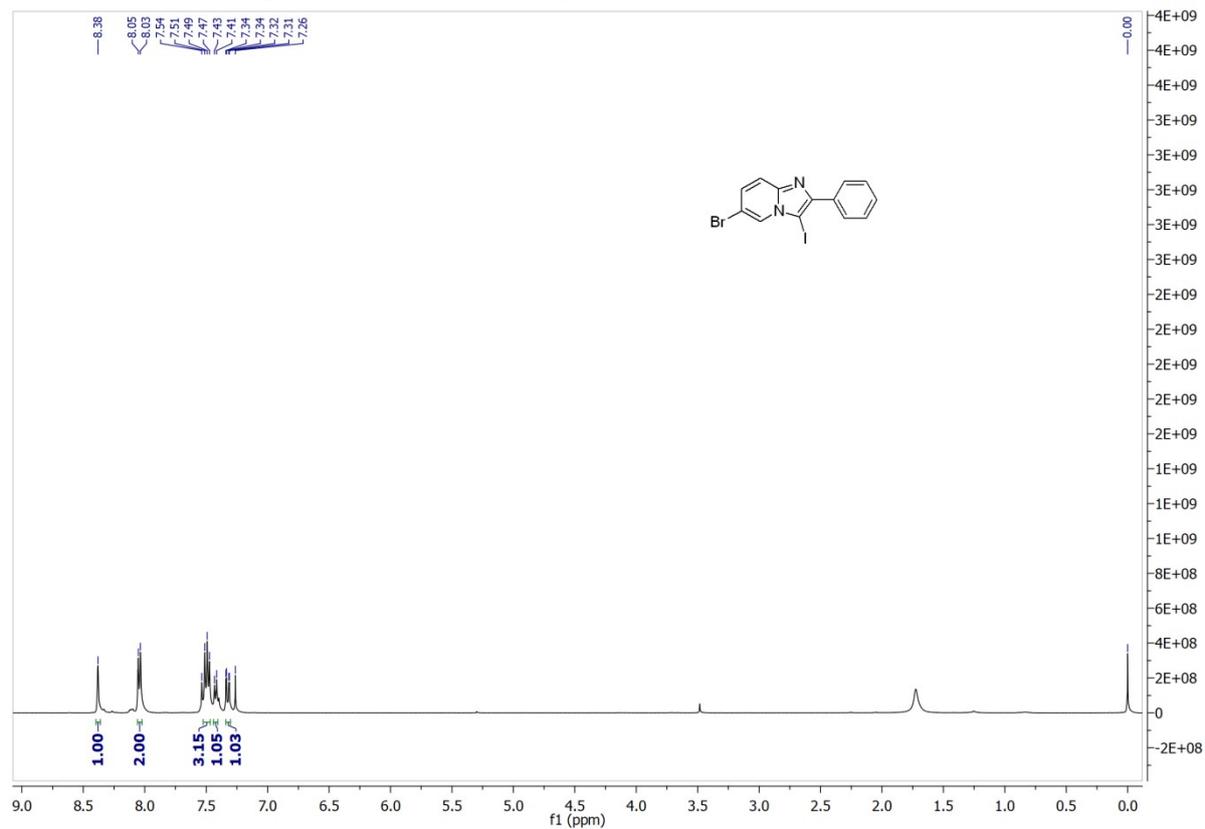
### 3-Iodo-7-methyl-2-phenylimidazo[1,2-a]pyridine (2c)



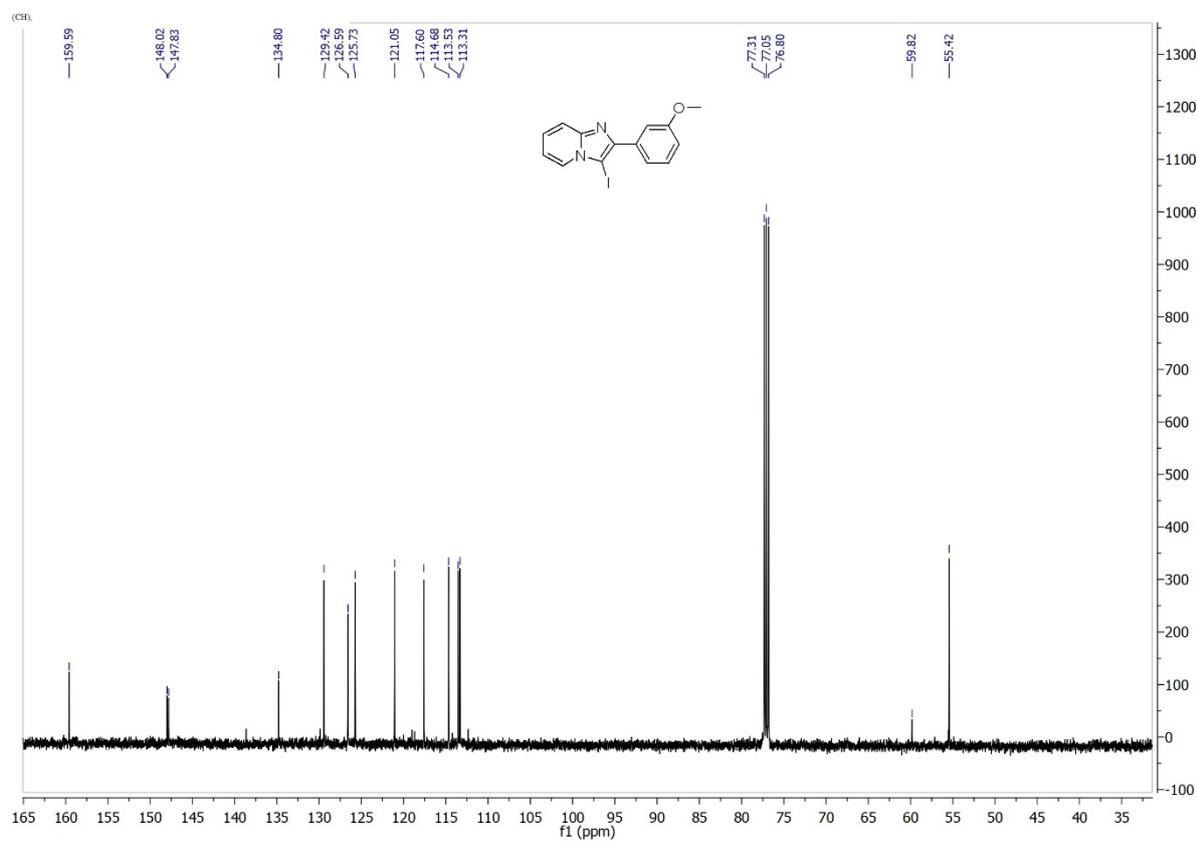
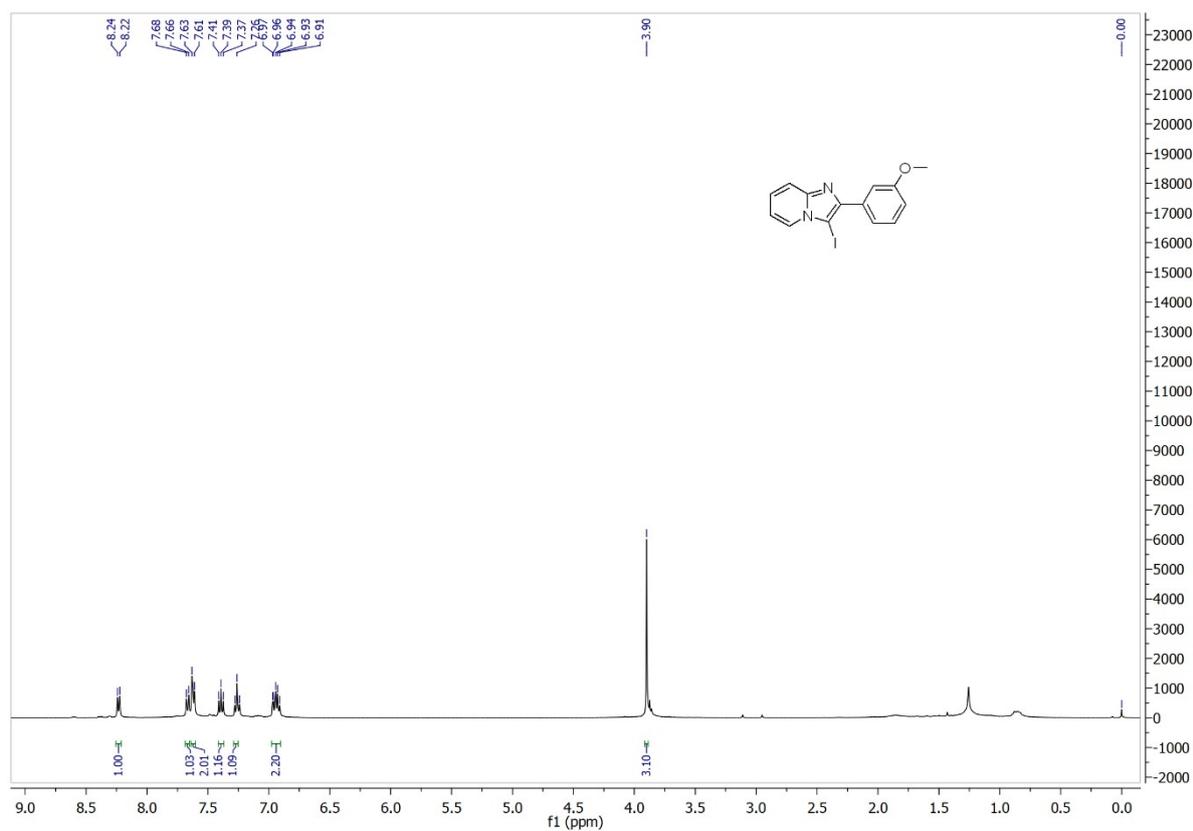
### 6-Chloro-3-iodo-2-phenylimidazo[1,2-a]pyridine (2d):



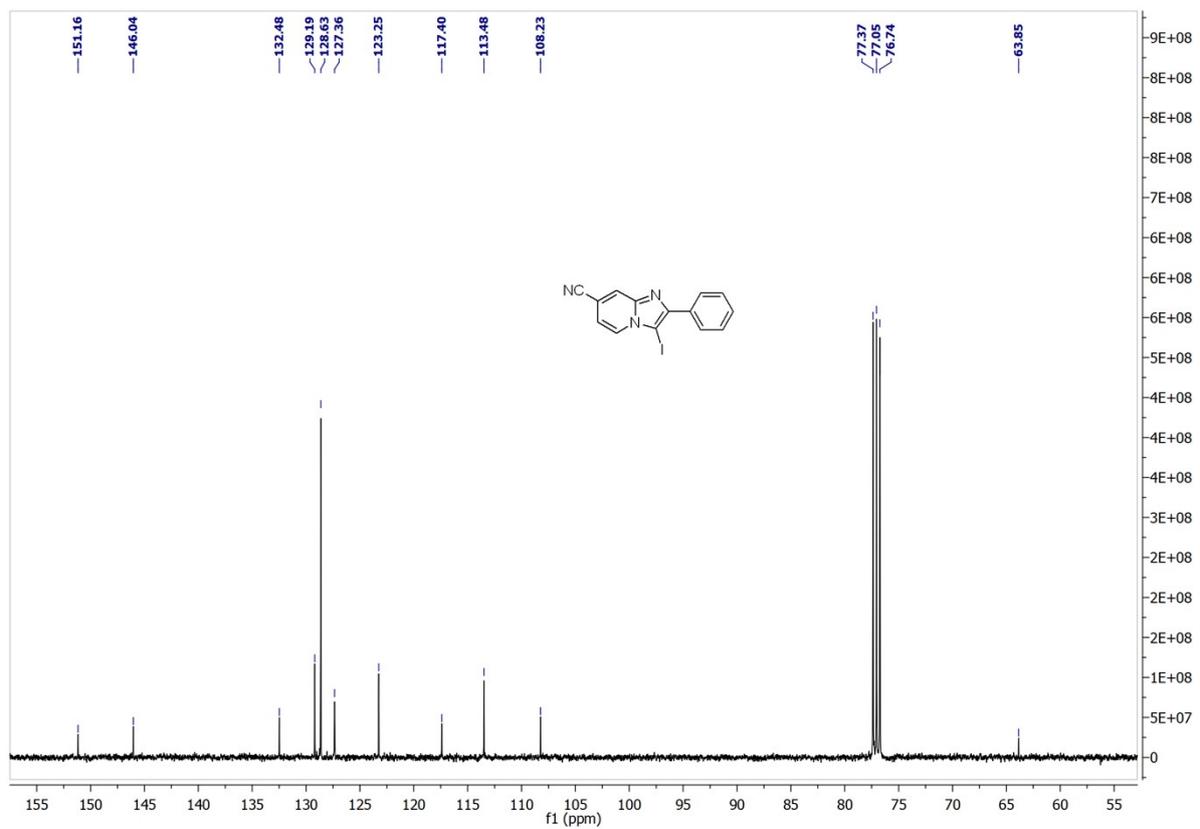
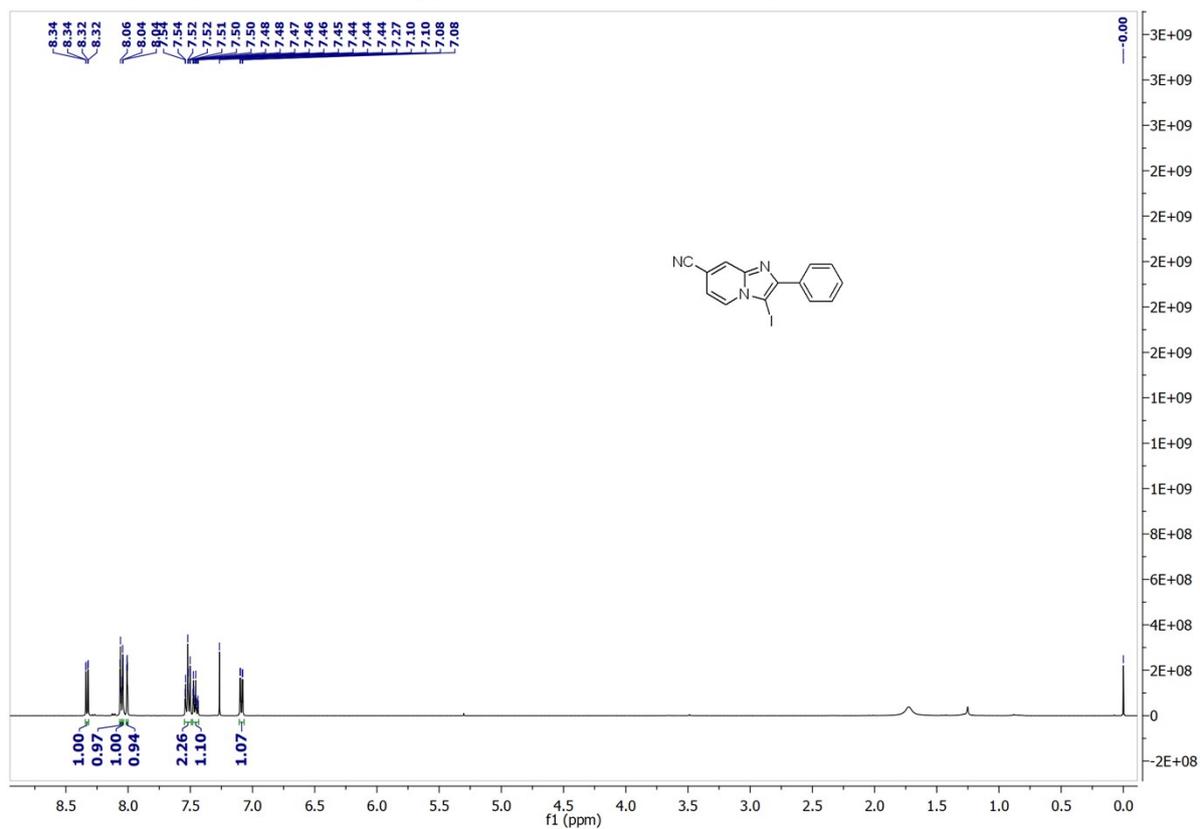
### 6-Bromo-3-iodo-2-phenylimidazo[1,2-a]pyridine (2e):



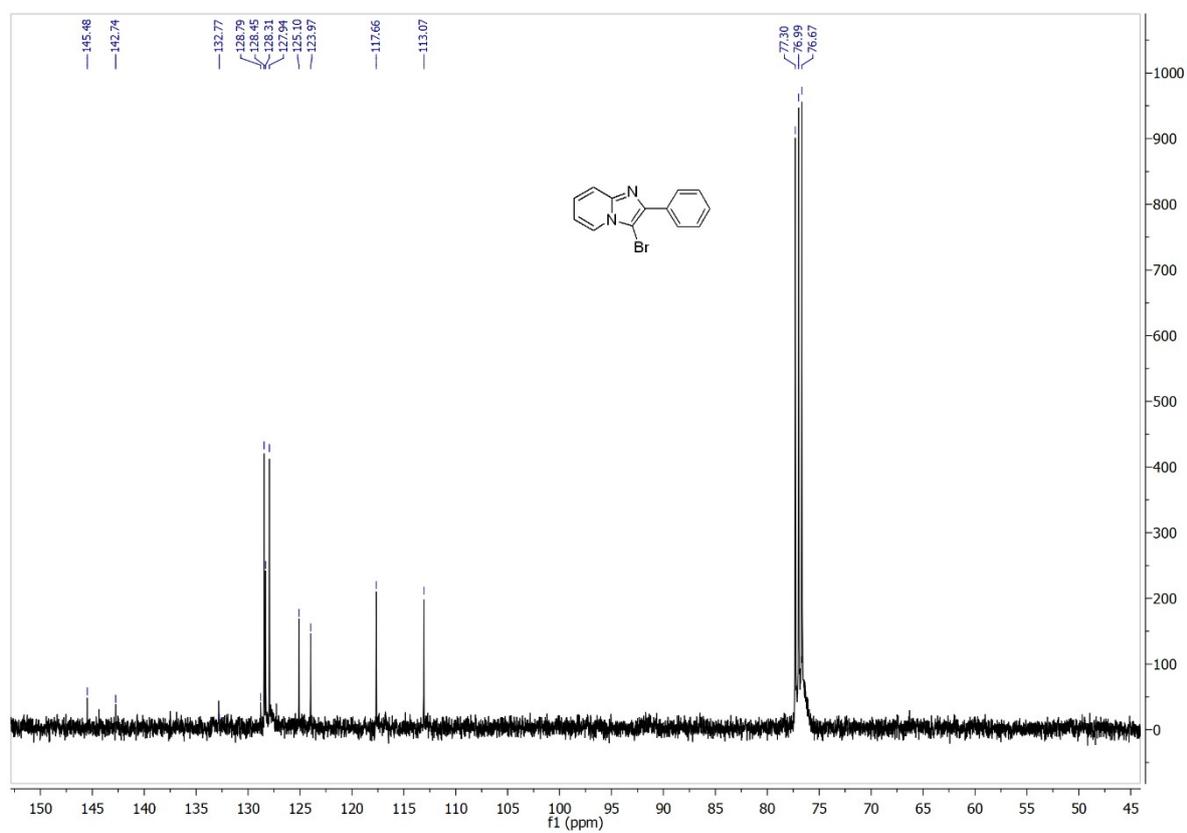
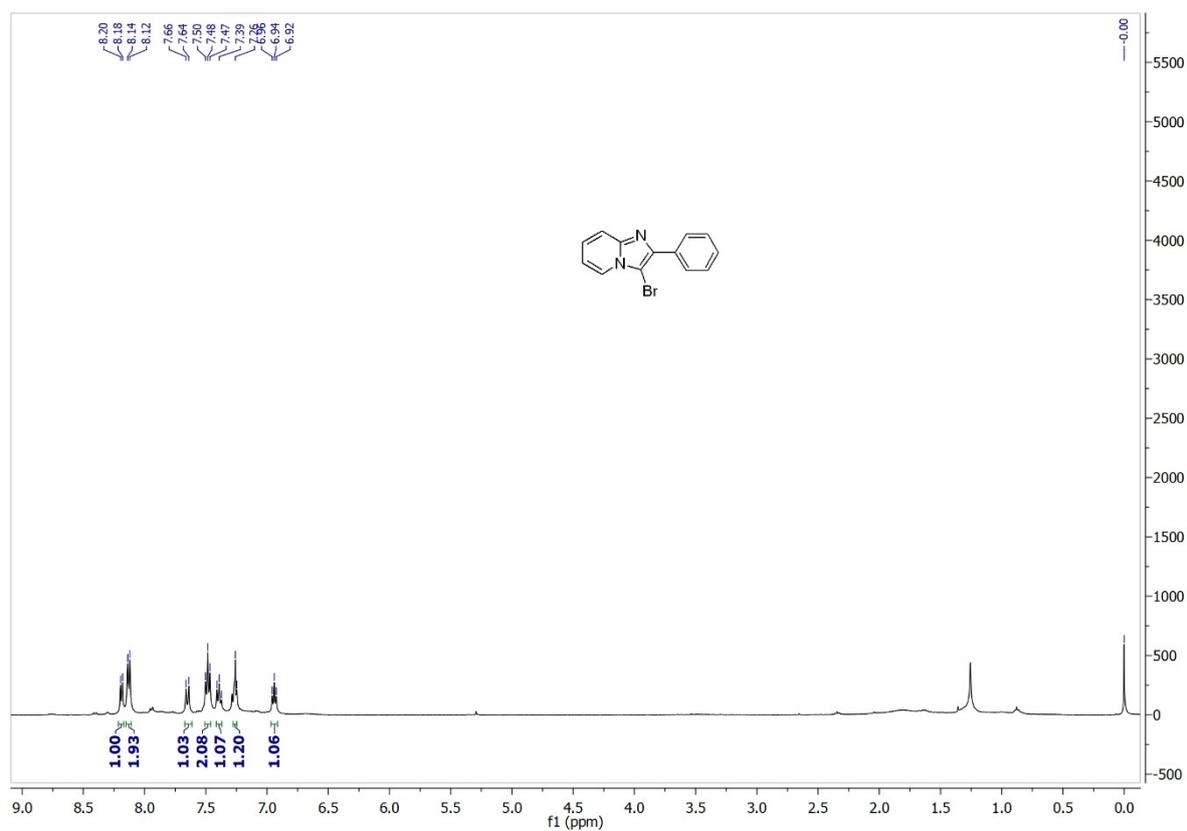
### 3-Iodo-2-(3-methoxyphenyl)imidazo[1,2-a]pyridine (2f):



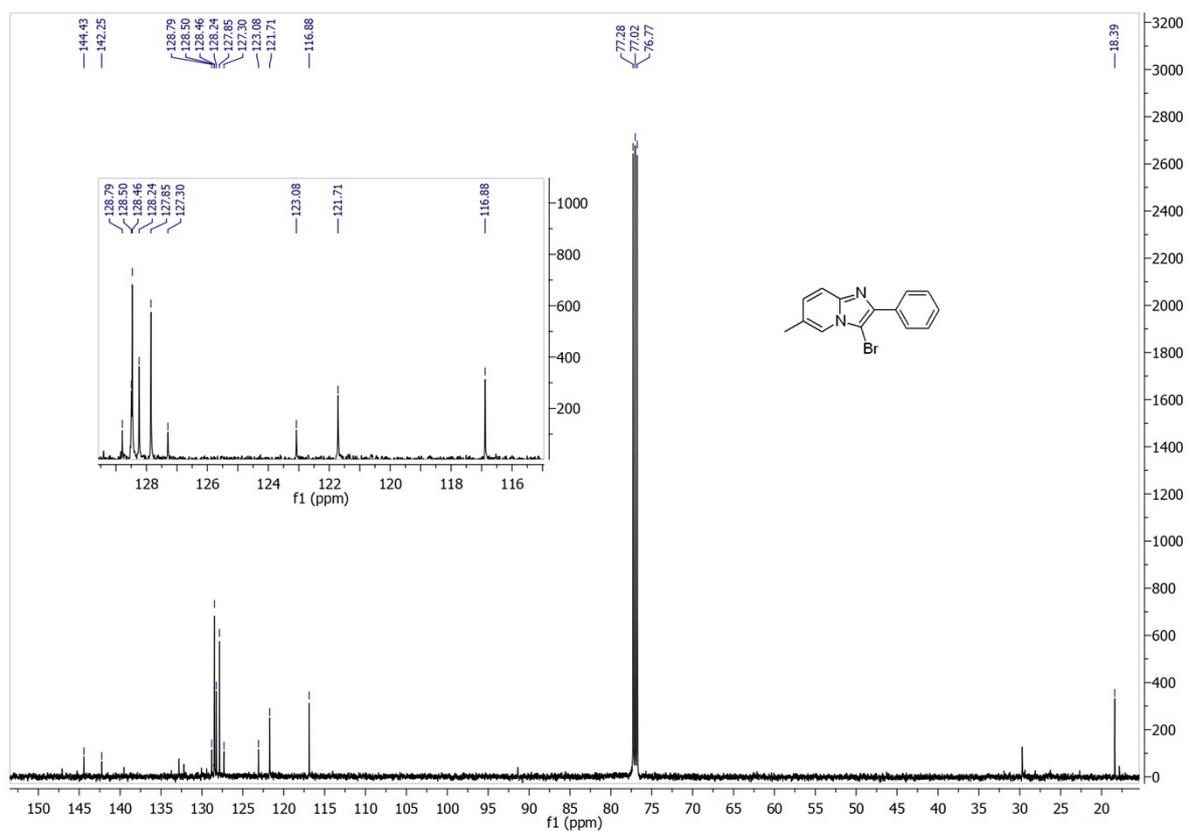
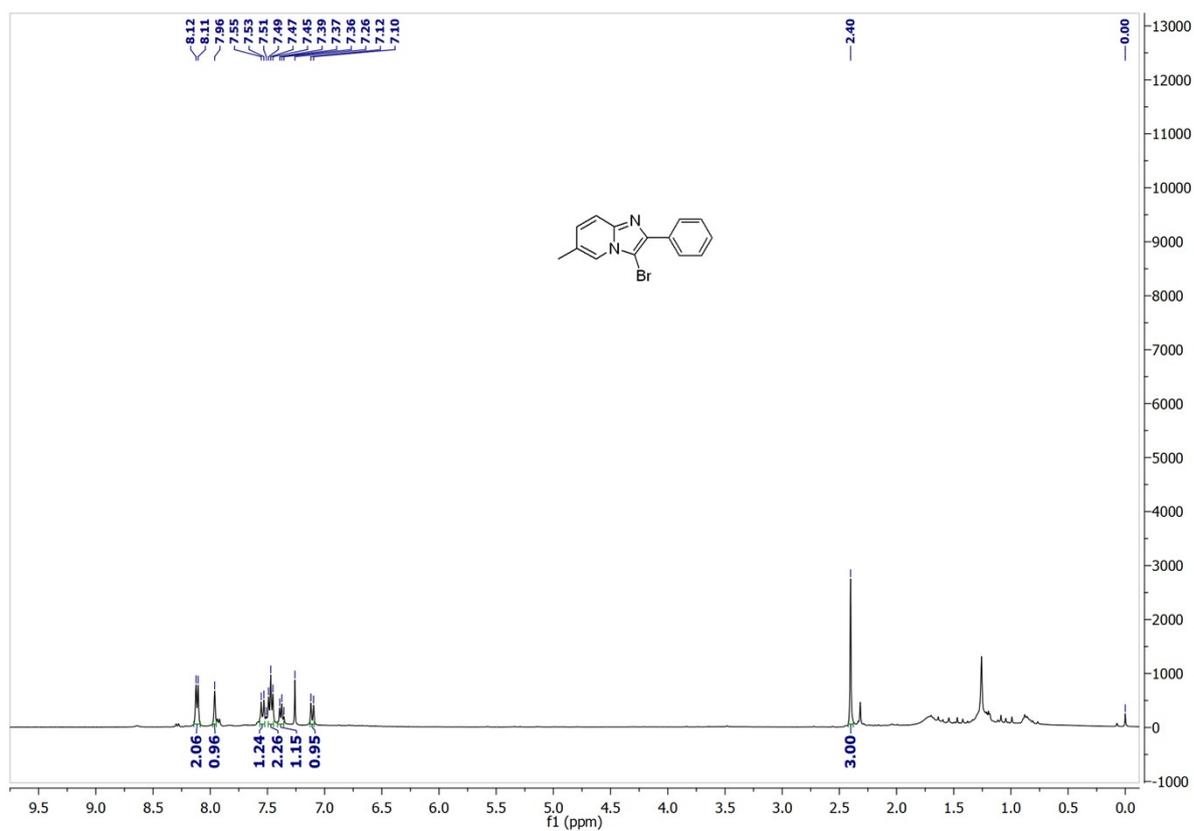
### 3-Iodo-2-phenylimidazo[1,2-a]pyridine-7-carbonitrile (2g):



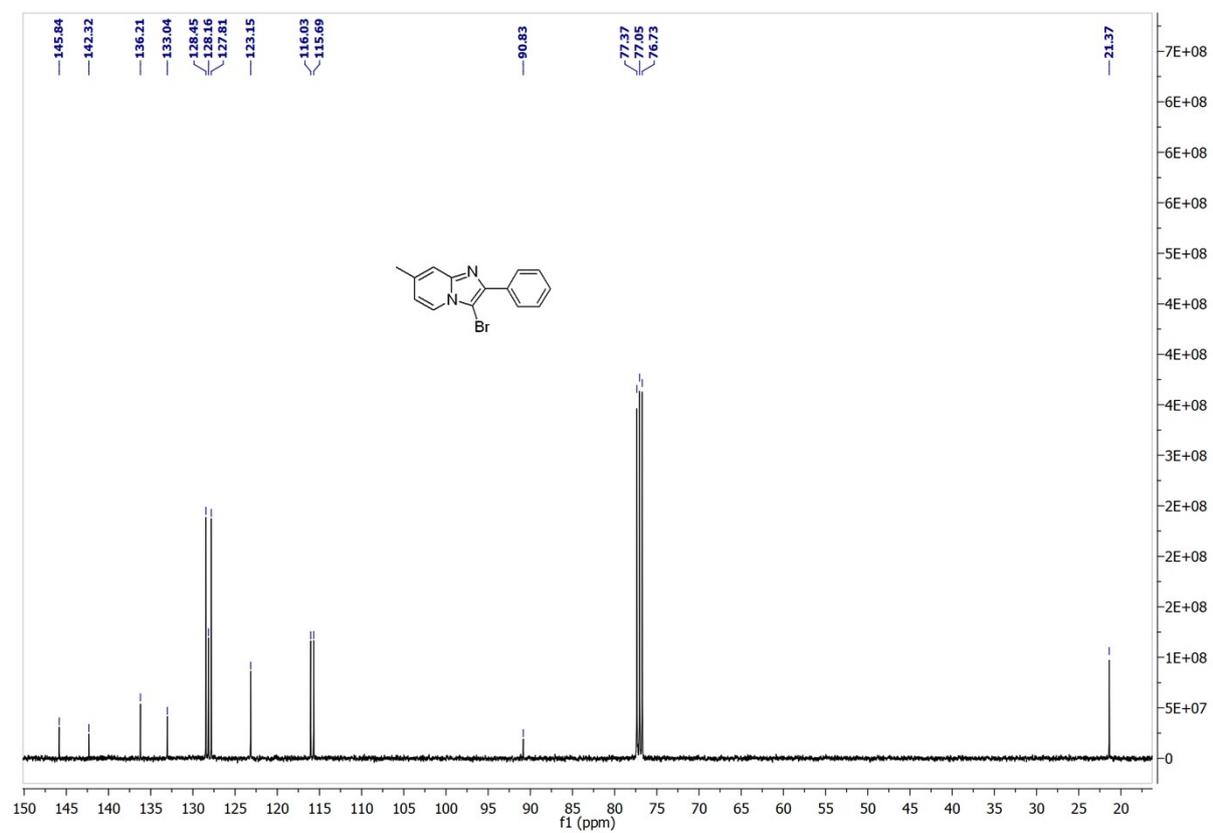
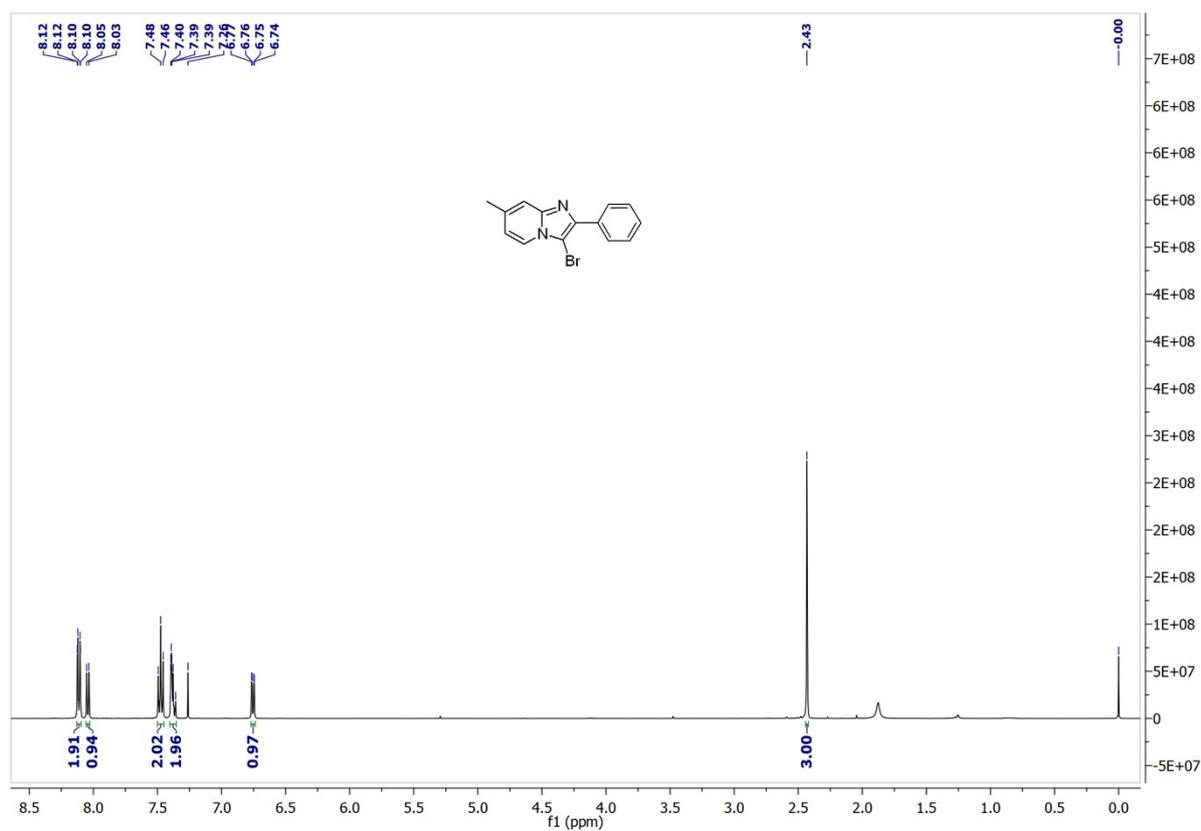
### 3-Bromo-2-phenylimidazo[1,2-a]pyridine (2h):



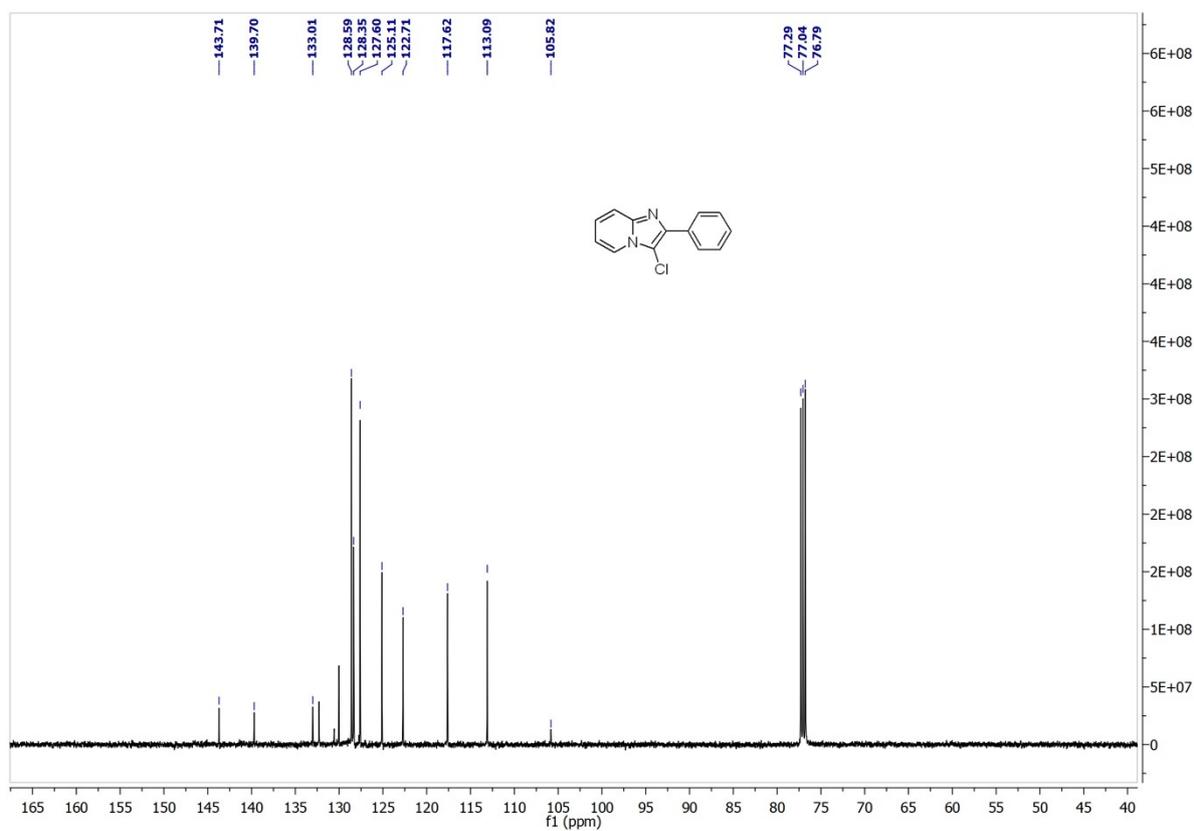
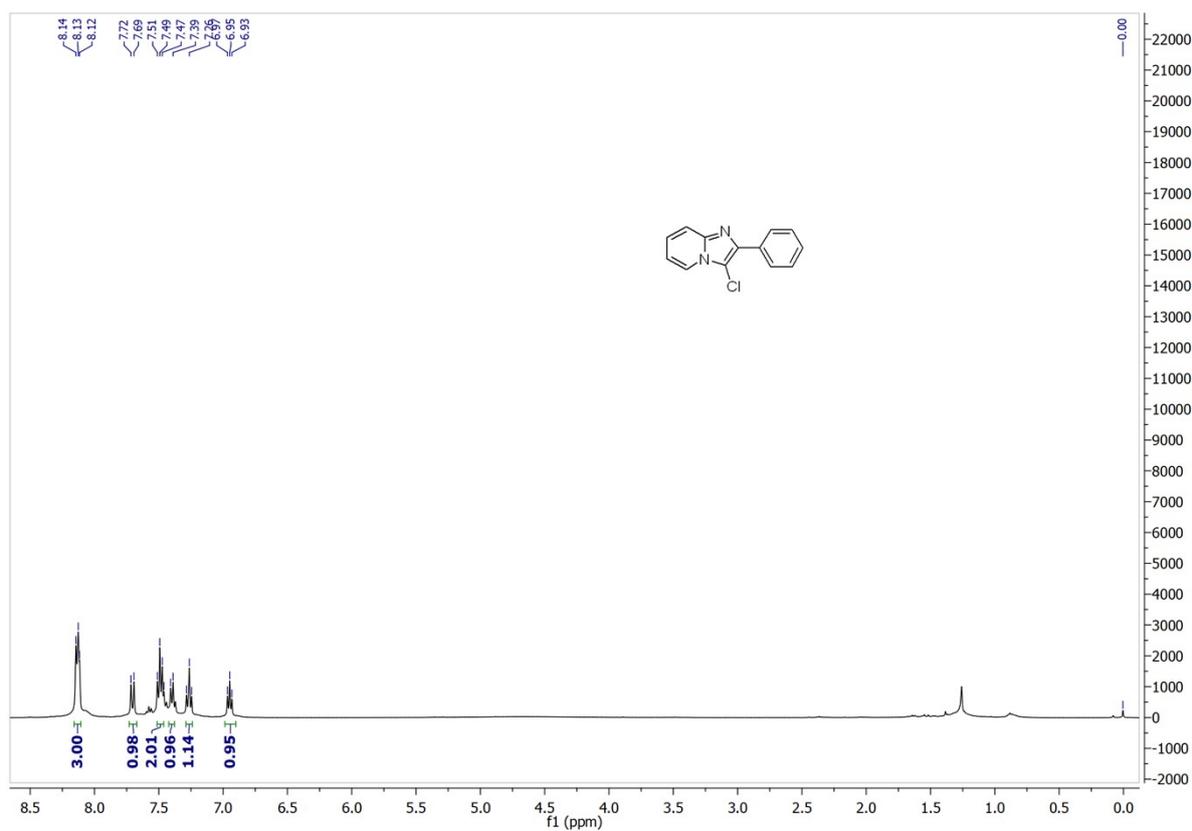
### 3-Bromo-6-methyl-2-phenylimidazo[1,2-a]pyridine (2i)



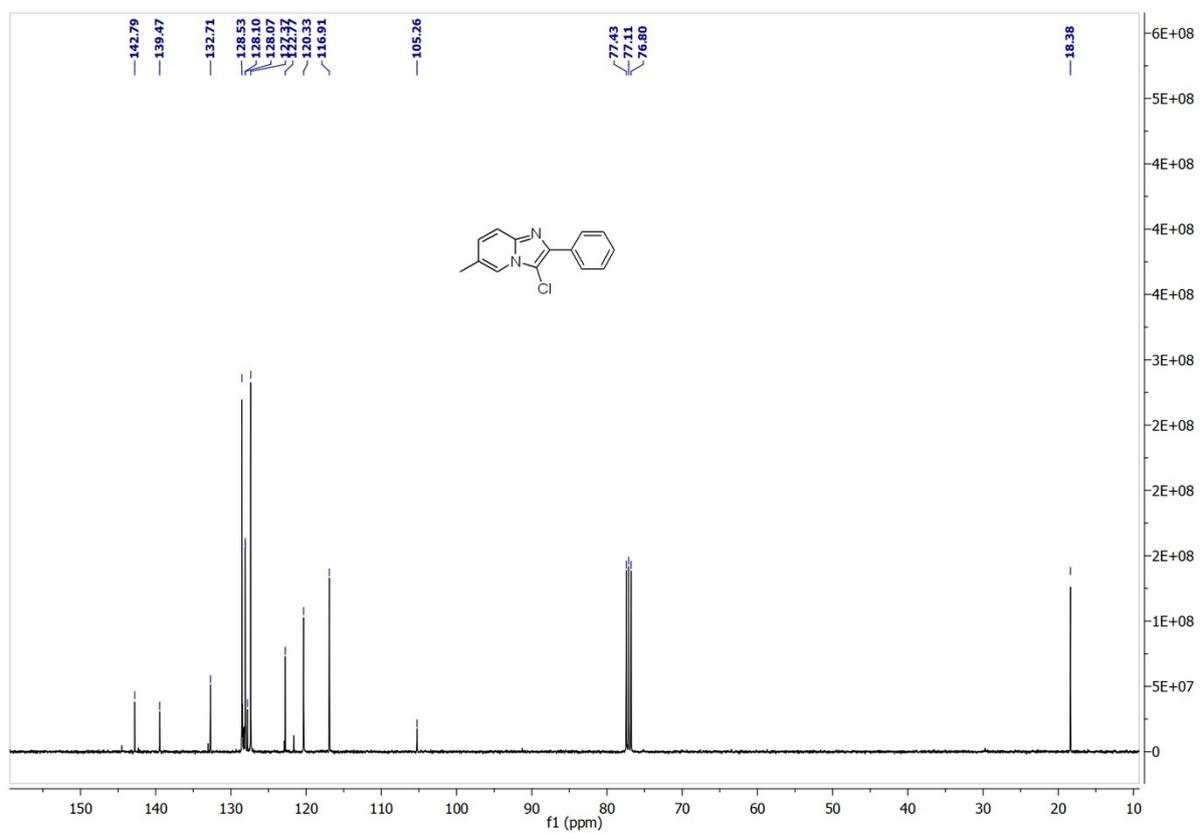
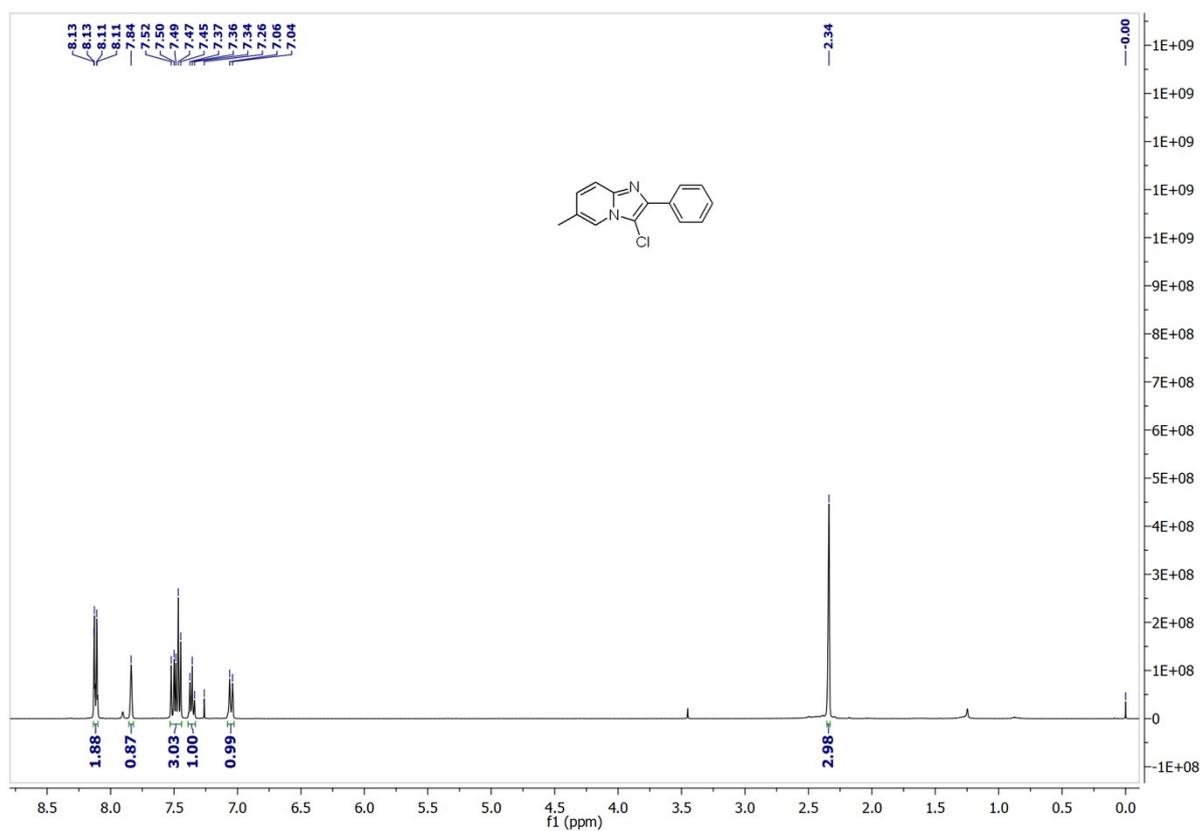
### 3-Bromo-7-methyl-2-phenylimidazo[1,2-a]pyridine (2j)



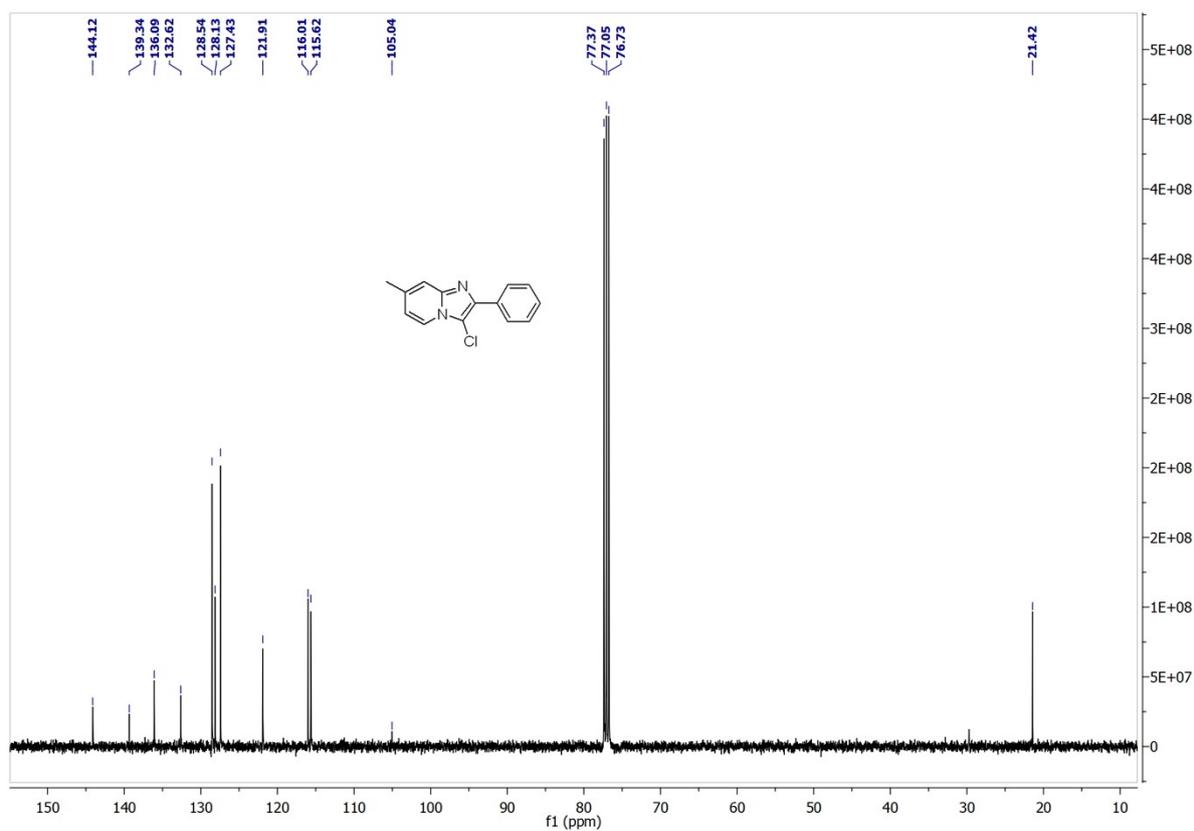
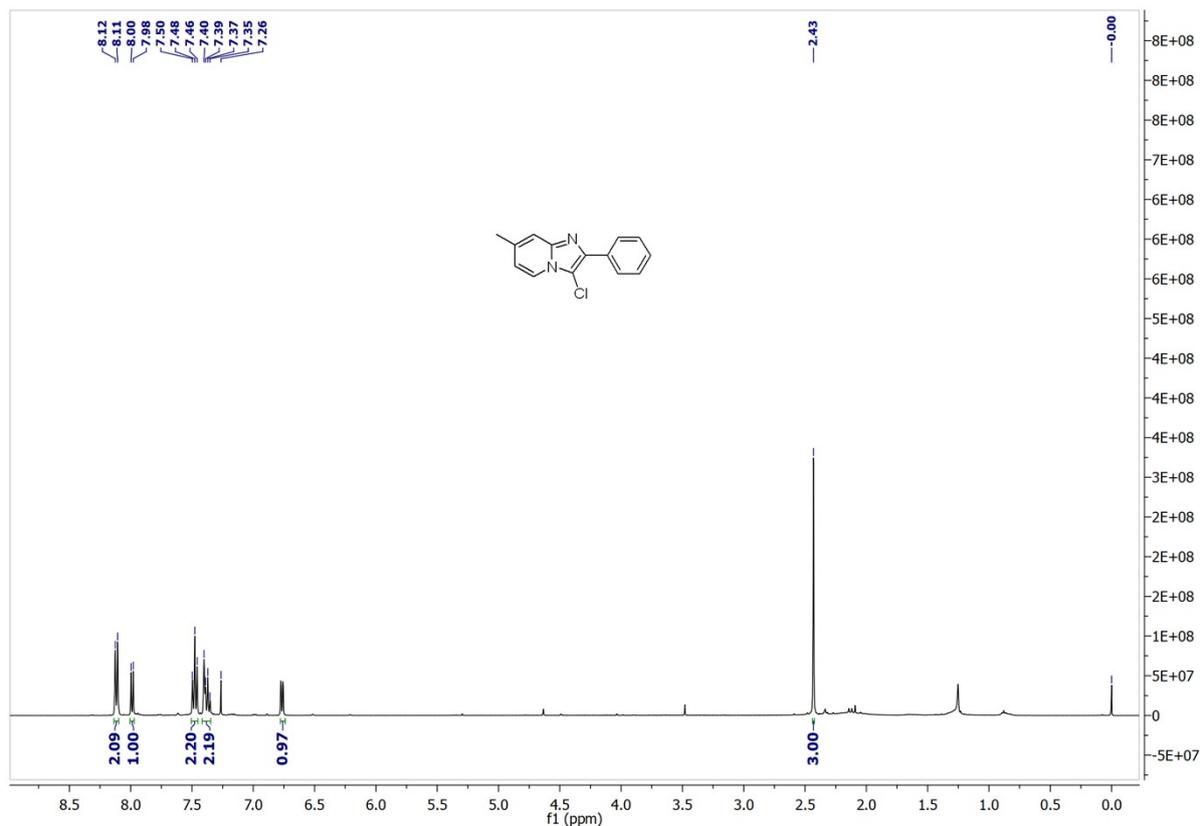
### 3-Chloro-2-phenylimidazo[1,2-a]pyridine (2k):



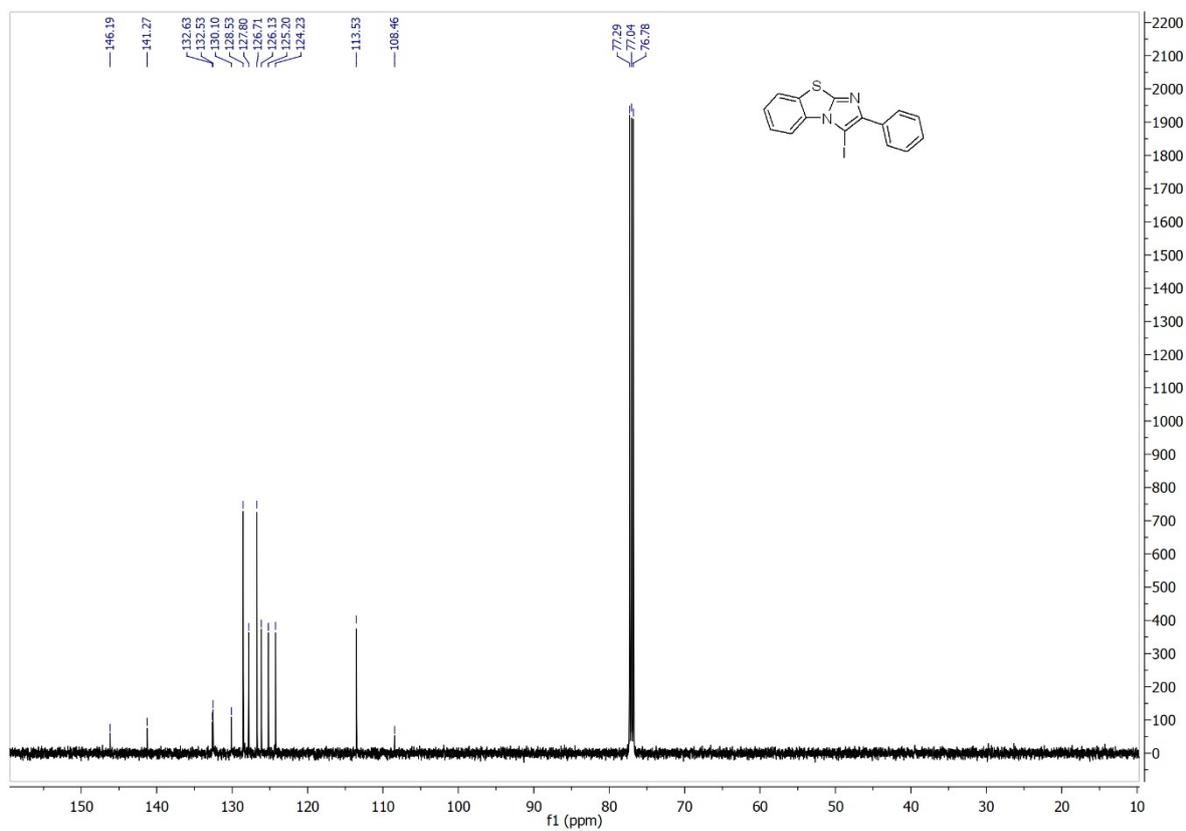
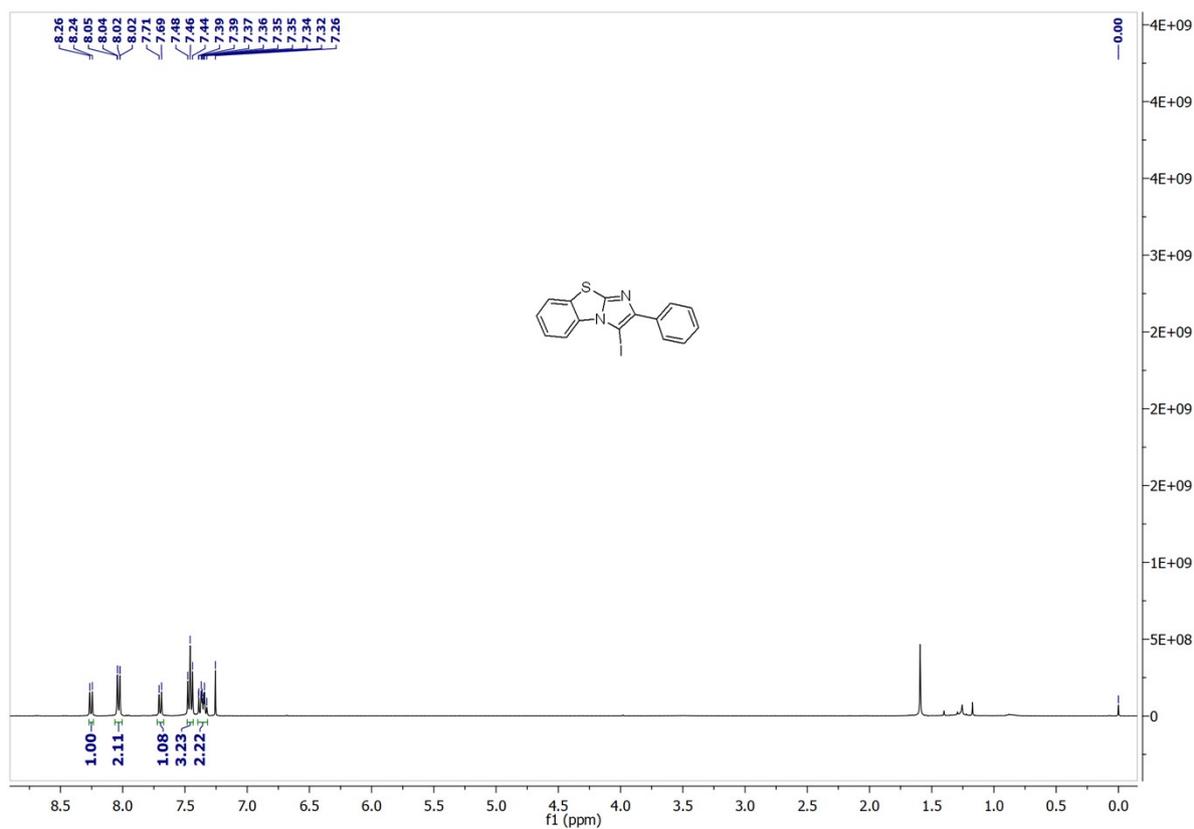
### 3-Chloro-6-methyl-2-phenylimidazo[1,2-a]pyridine (2l):



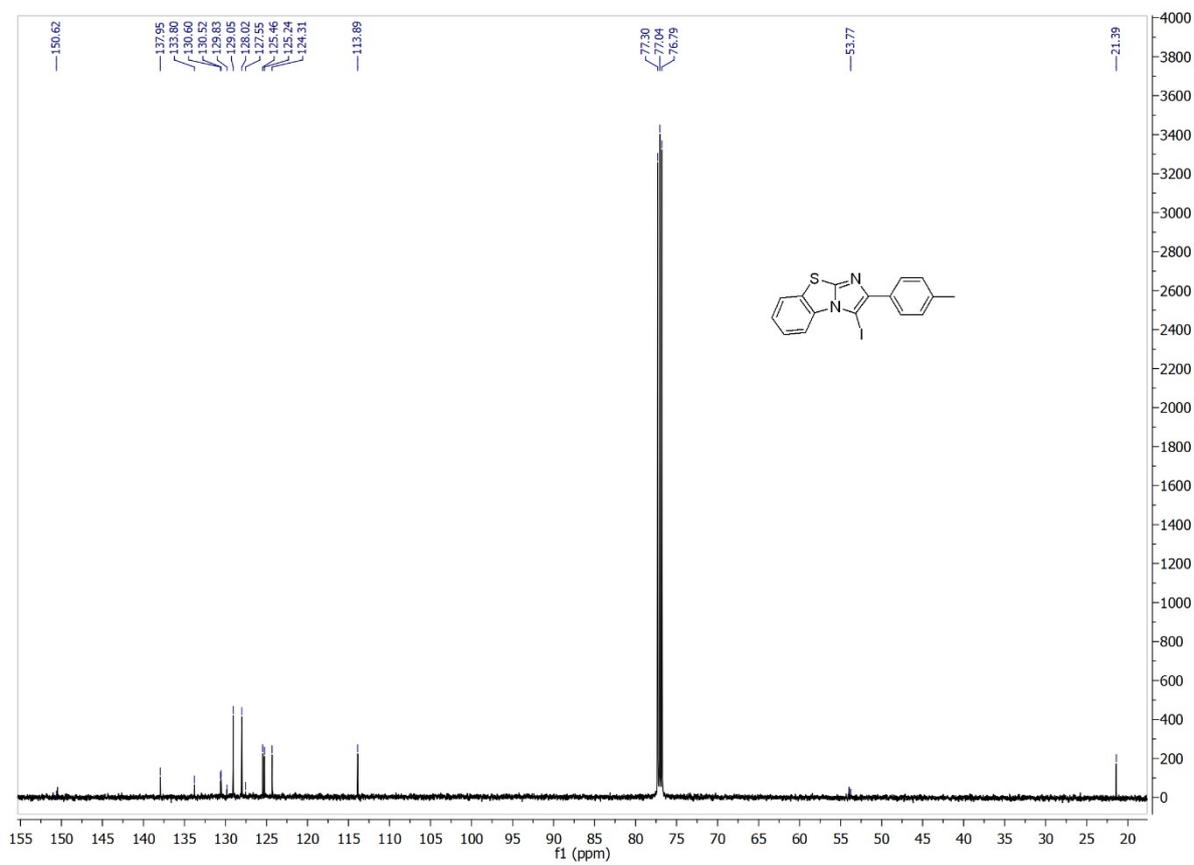
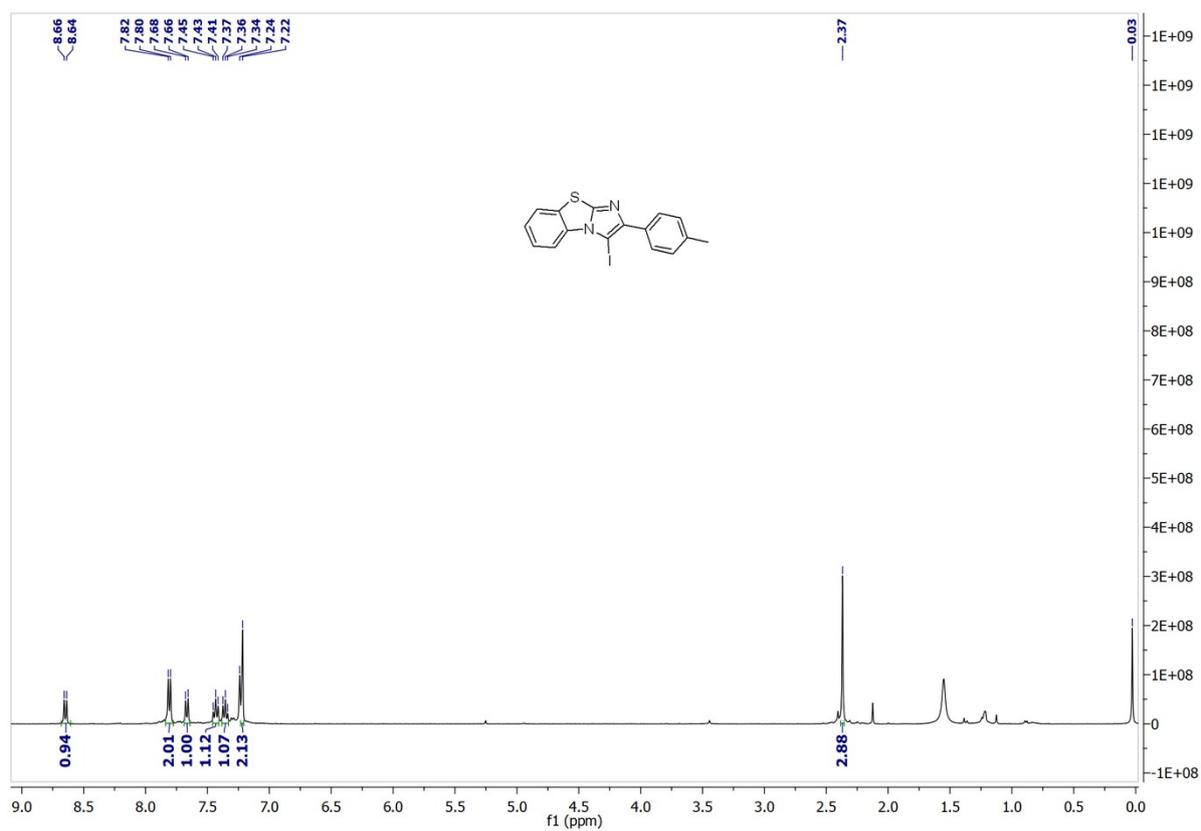
### 3-Chloro-7-methyl-2-phenylimidazo[1,2-a]pyridine (2m):



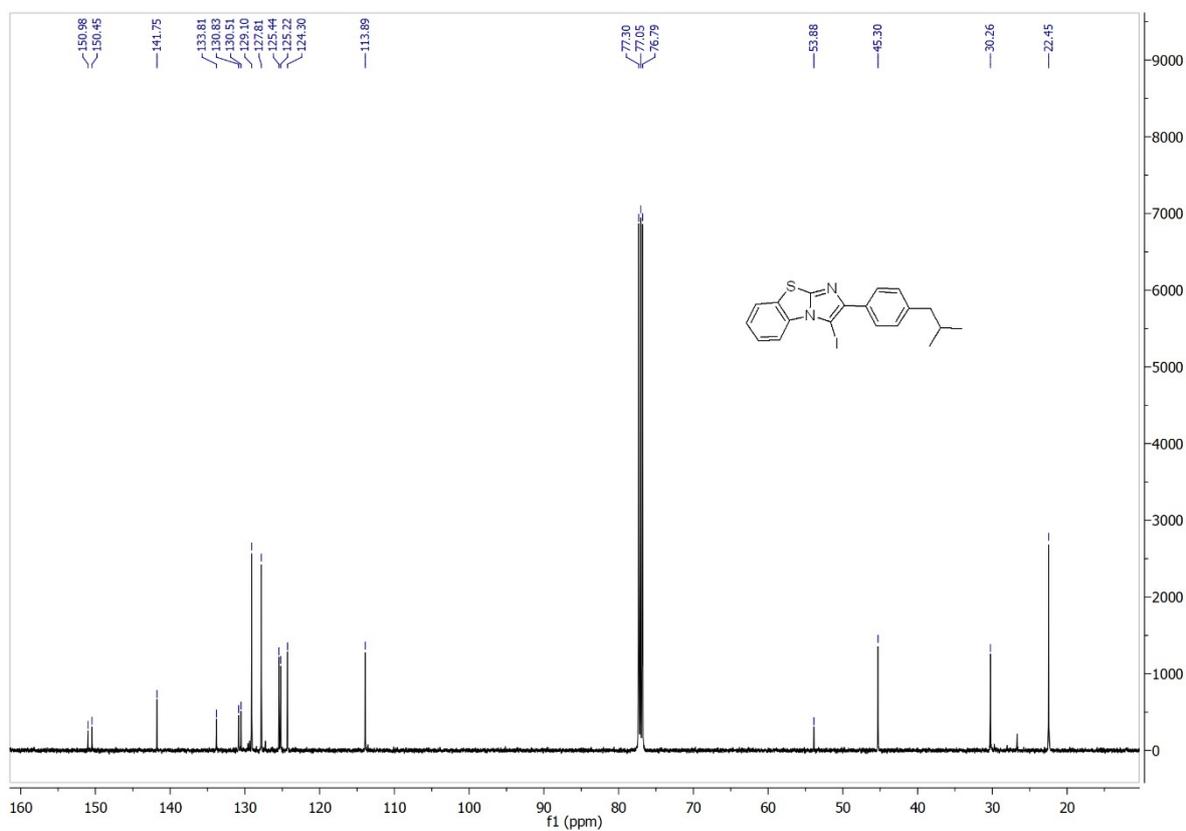
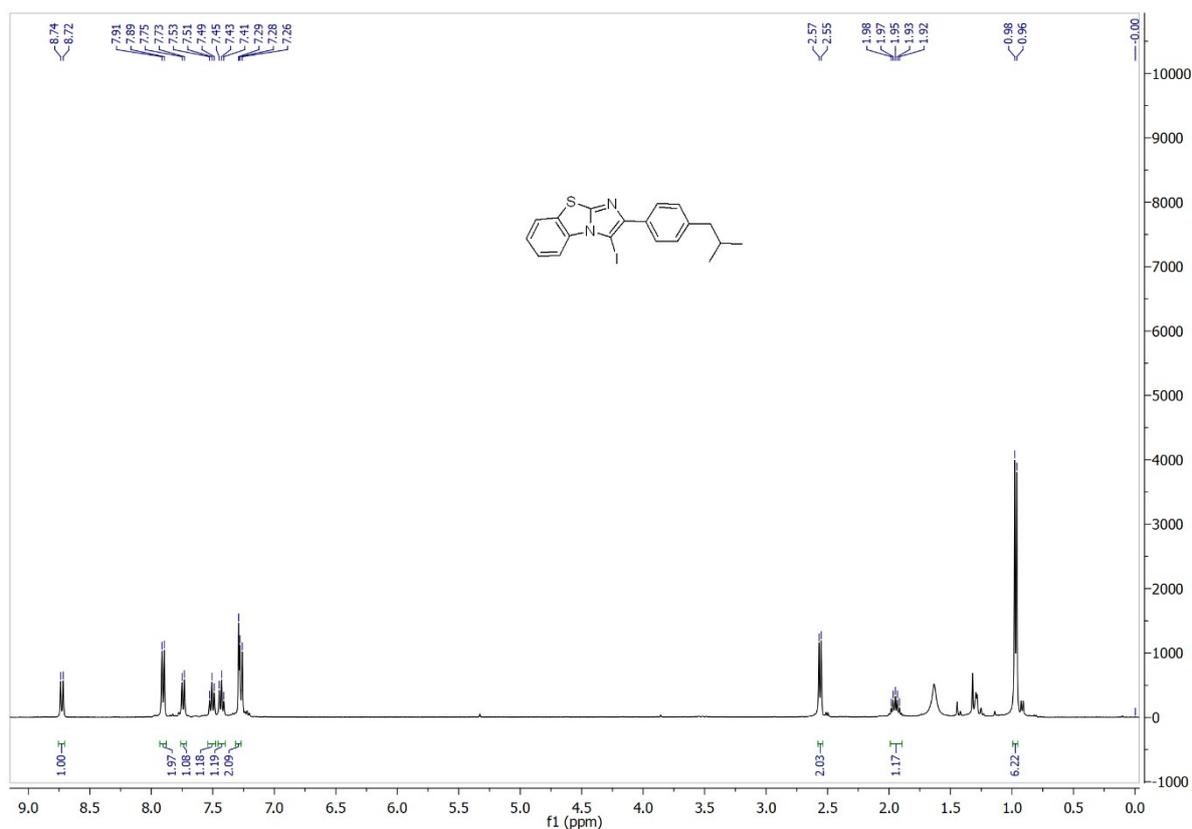
### 3-Iodo-2-phenylbenzo[d]imidazo[2,1-b]thiazole (6a):



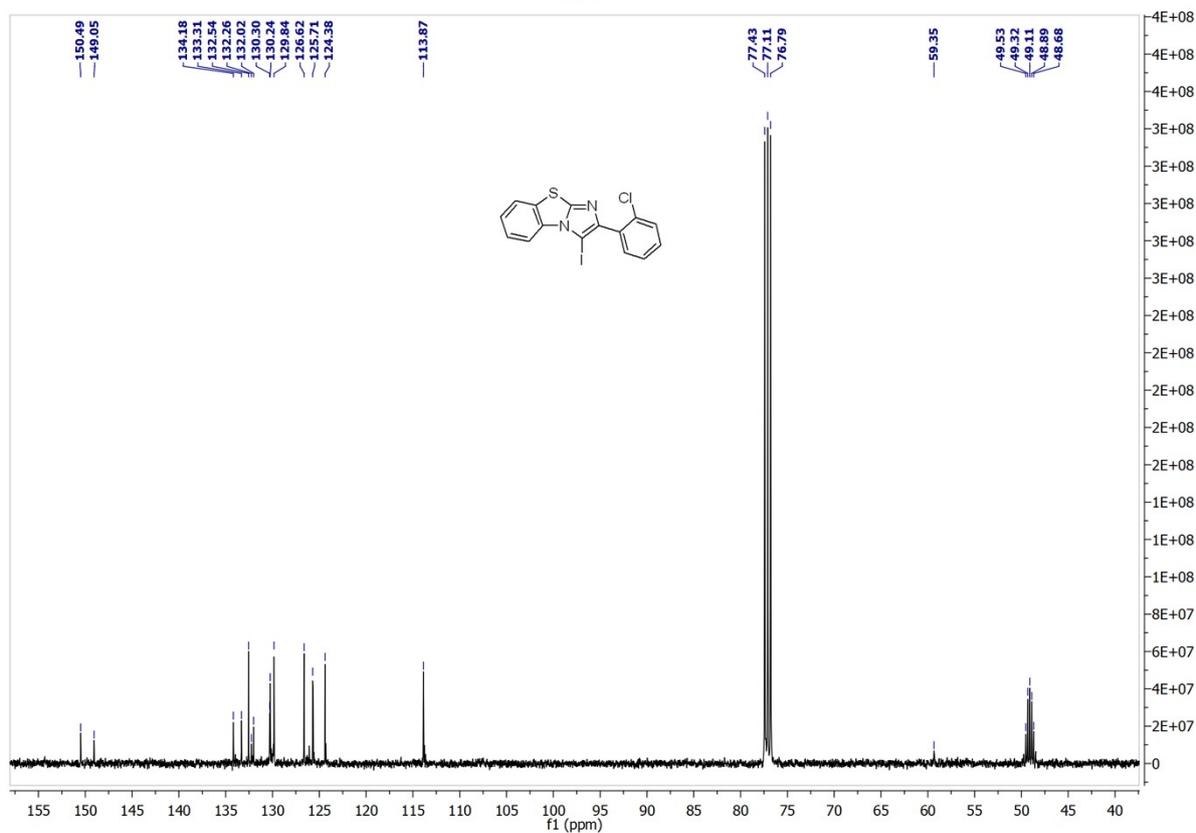
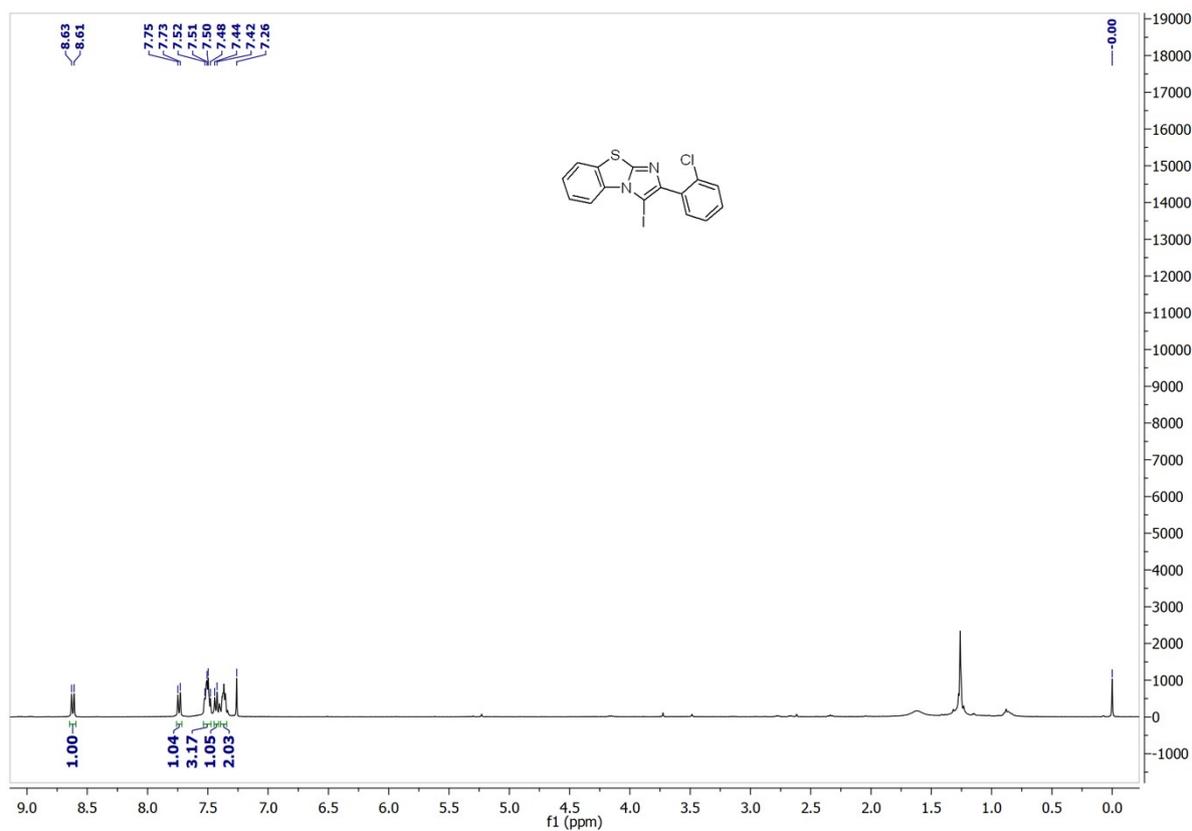
### 3-Iodo-2-(p-tolyl)benzo[d]imidazo[2,1-b]thiazole (6b)



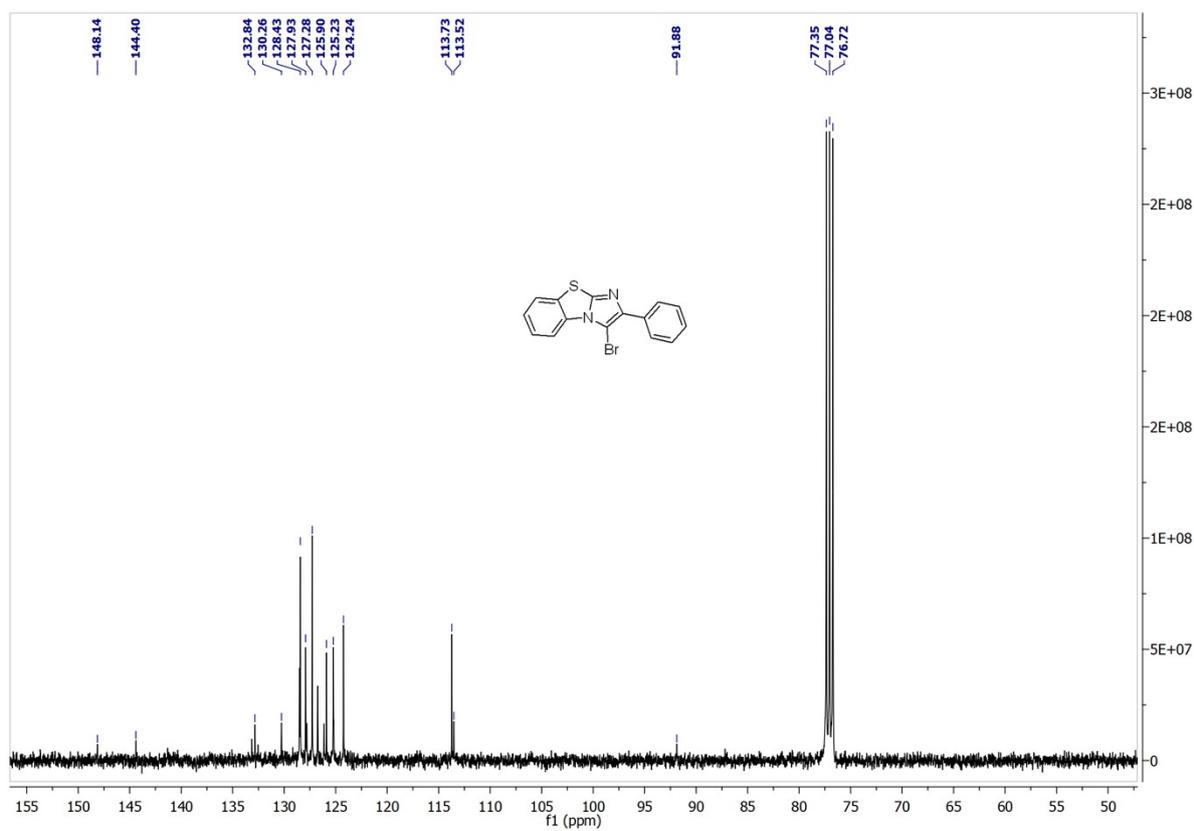
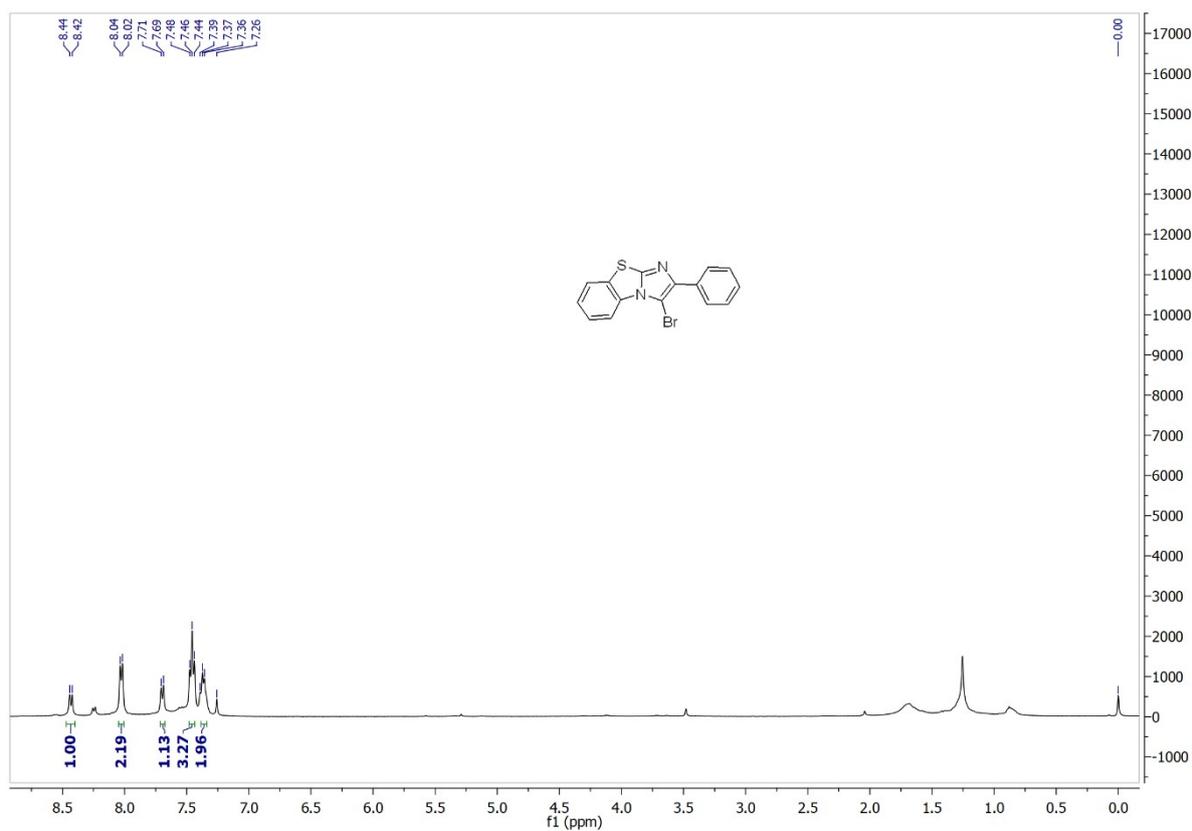
### 3-Iodo-2-(4-isobutylphenyl)benzo[d]imidazo[2,1-b]-thiazole (6c)



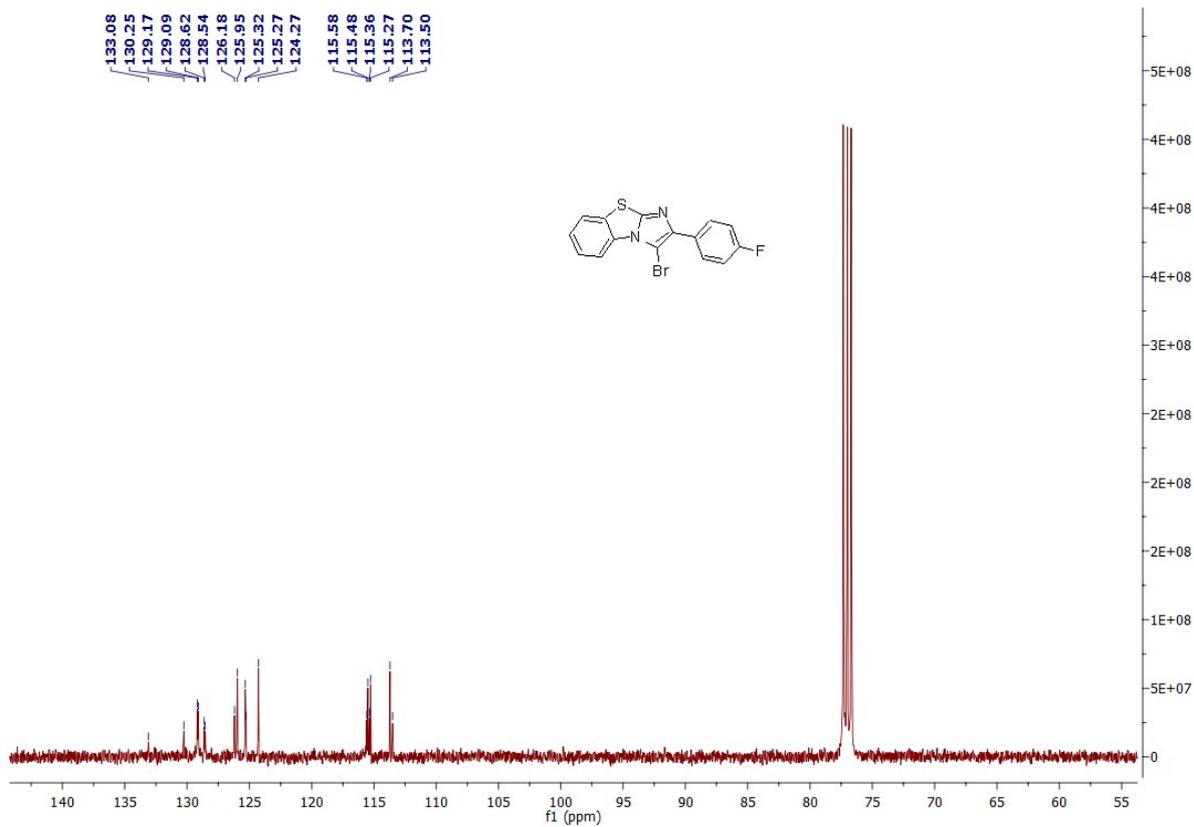
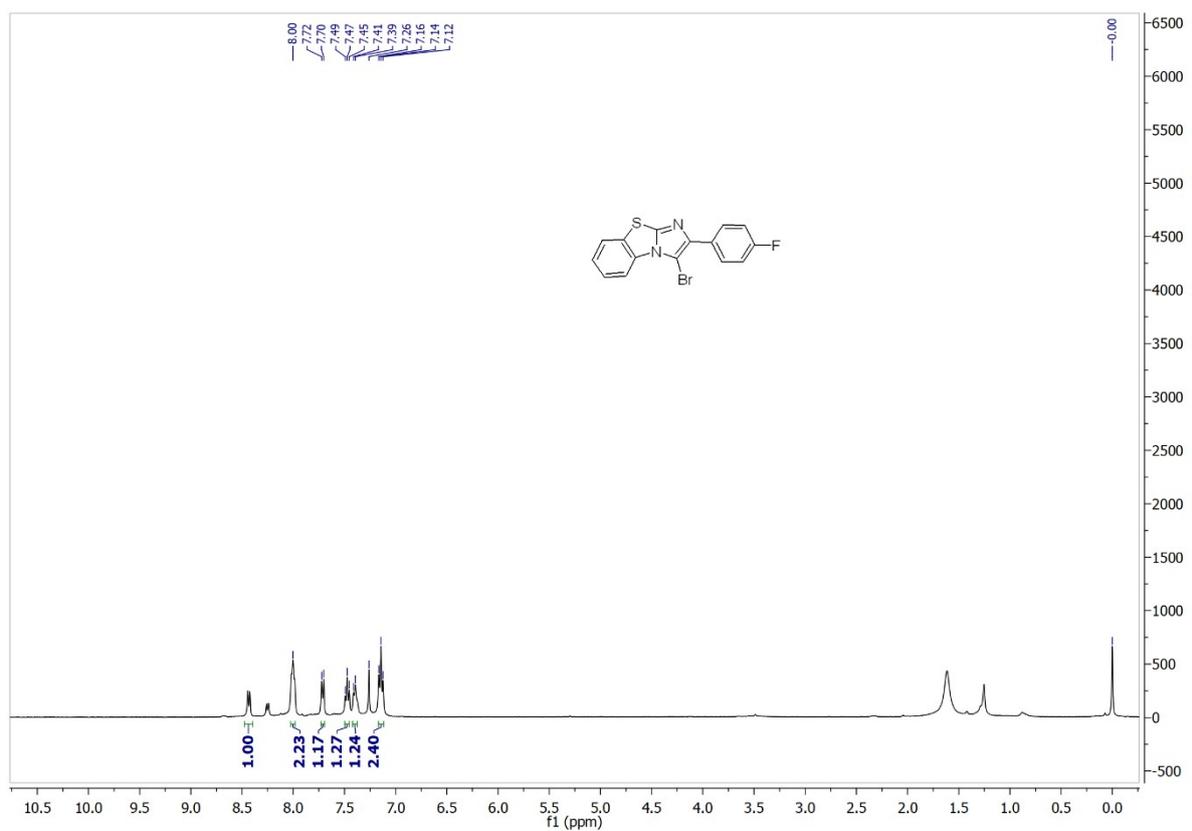
## 2-(2-Chlorophenyl)-3-iodobenzo[d]imidazo[2,1-b]thiazole(6d):



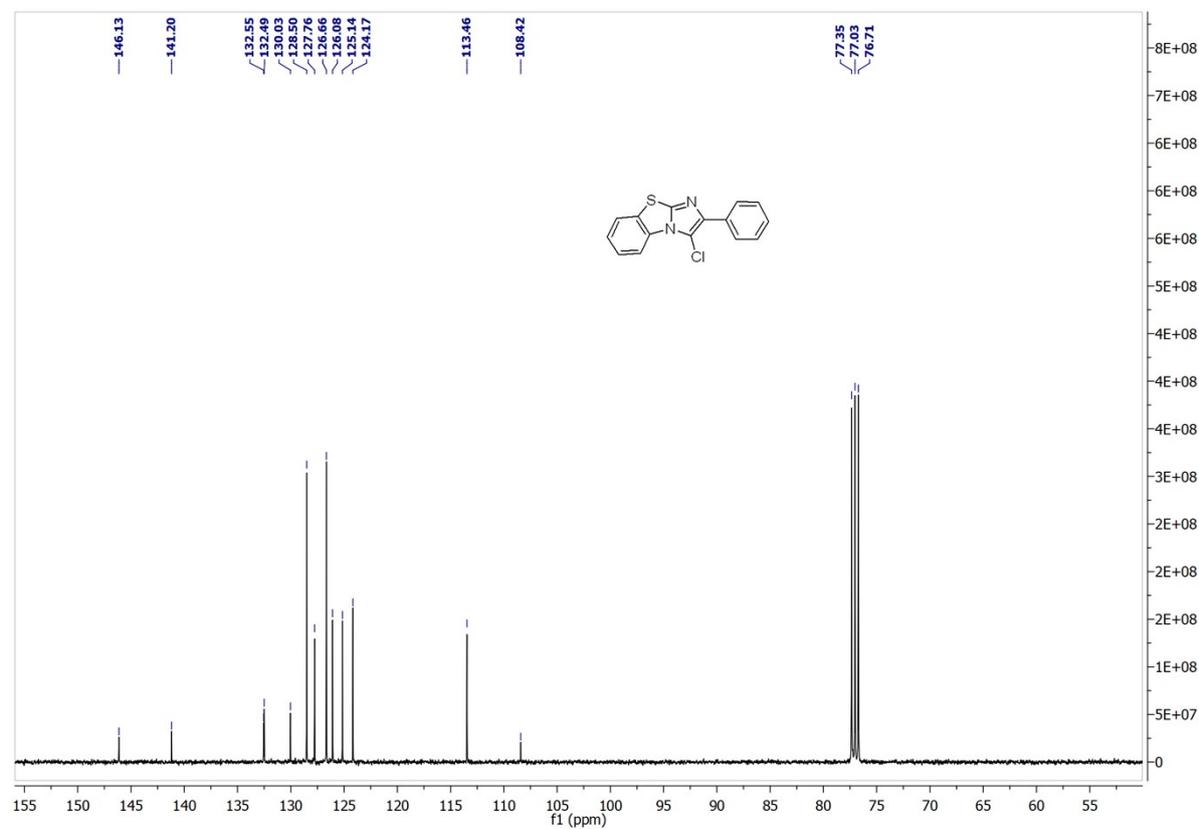
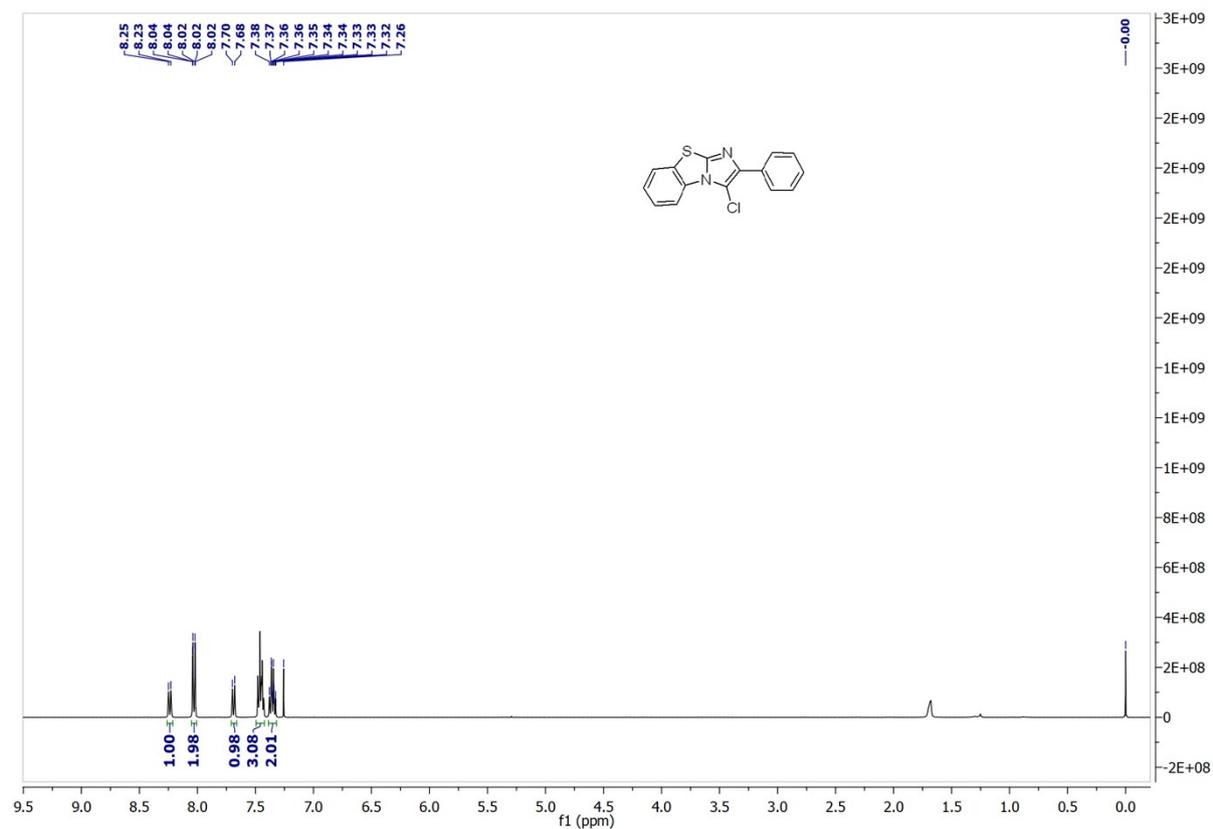
### 3-Bromo-2-phenylbenzo[d]imidazo[2,1-b]thiazole (6e)



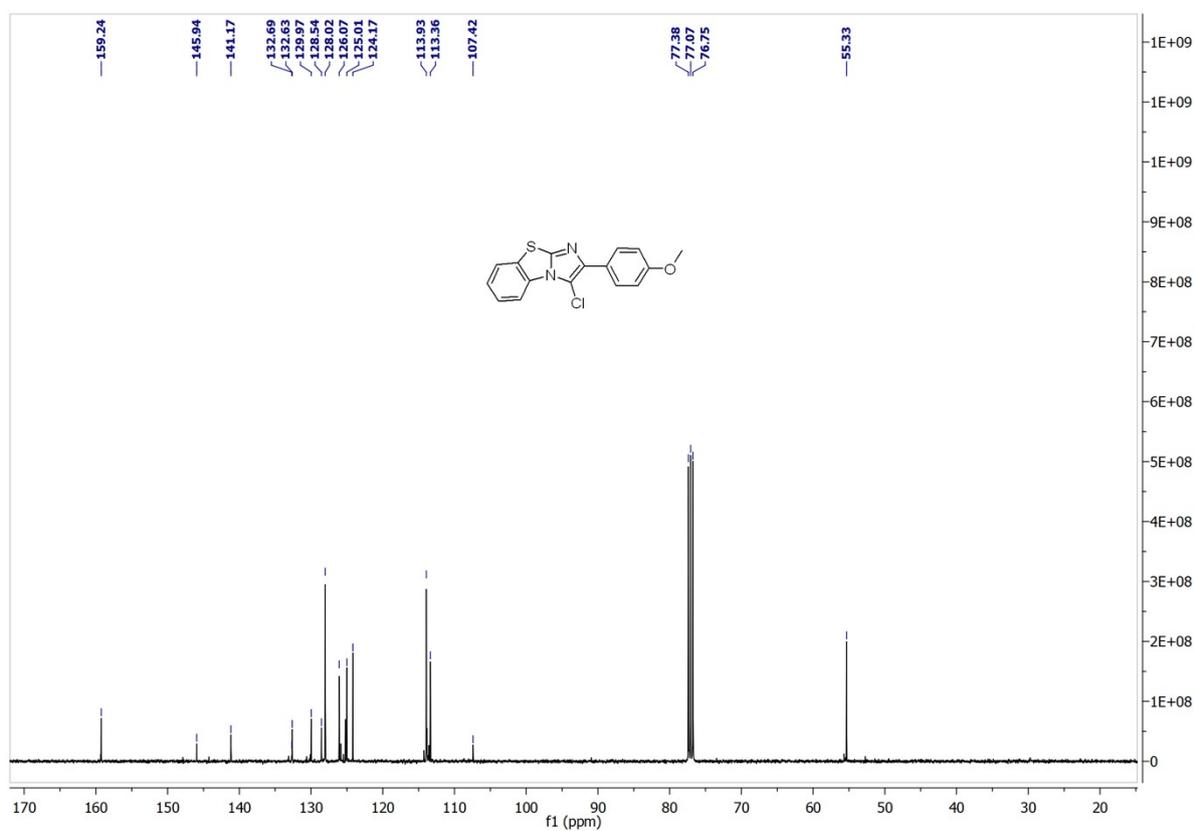
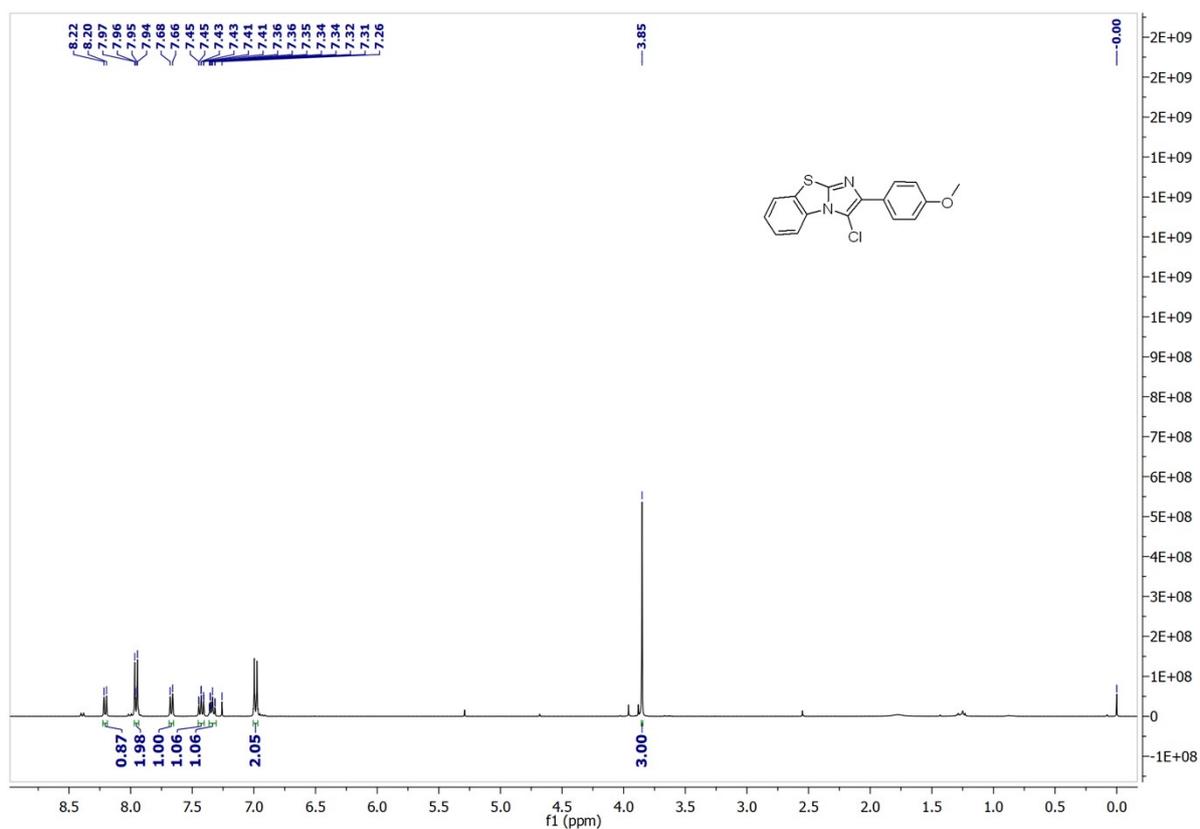
### 3-Bromo-2-(4-fluorophenyl)benzo[d]imidazo[2,1-b]thiazole (6f)



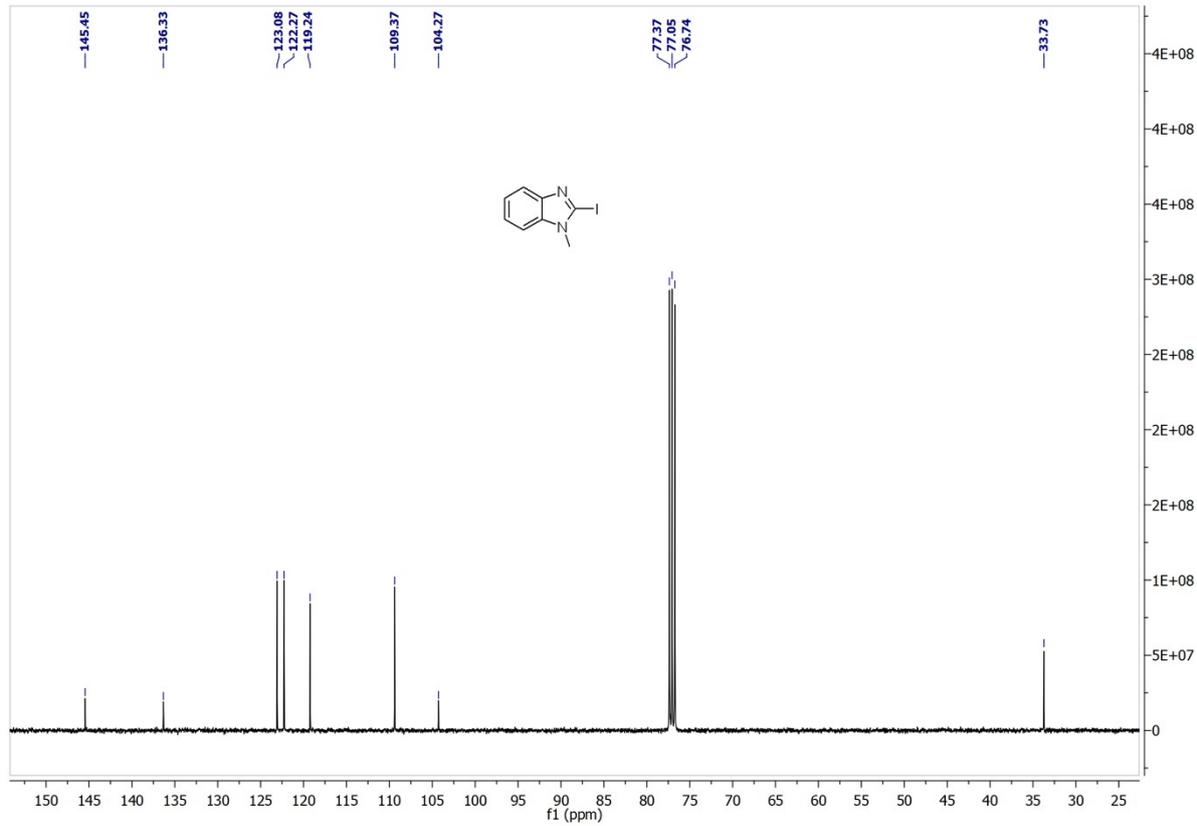
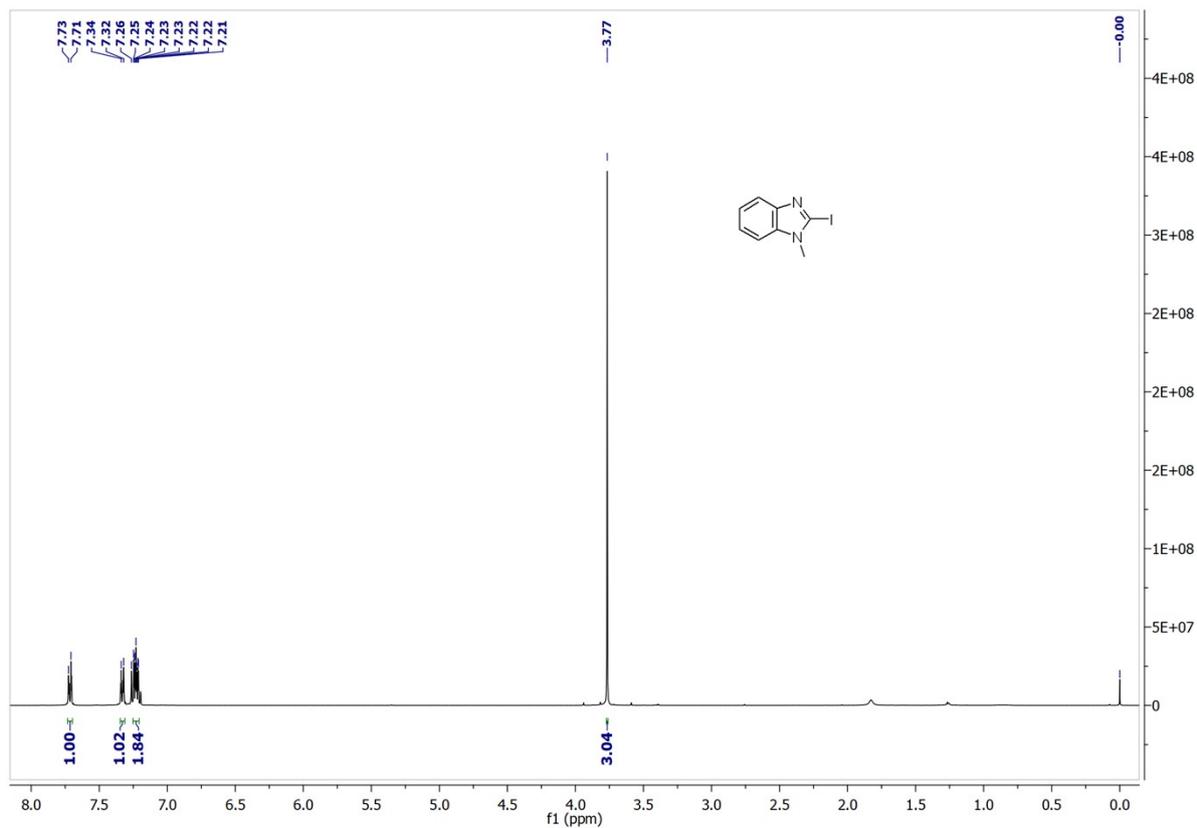
### 3-Chloro-2-phenylbenzo[d]imidazo[2,1-b]thiazole (6g):



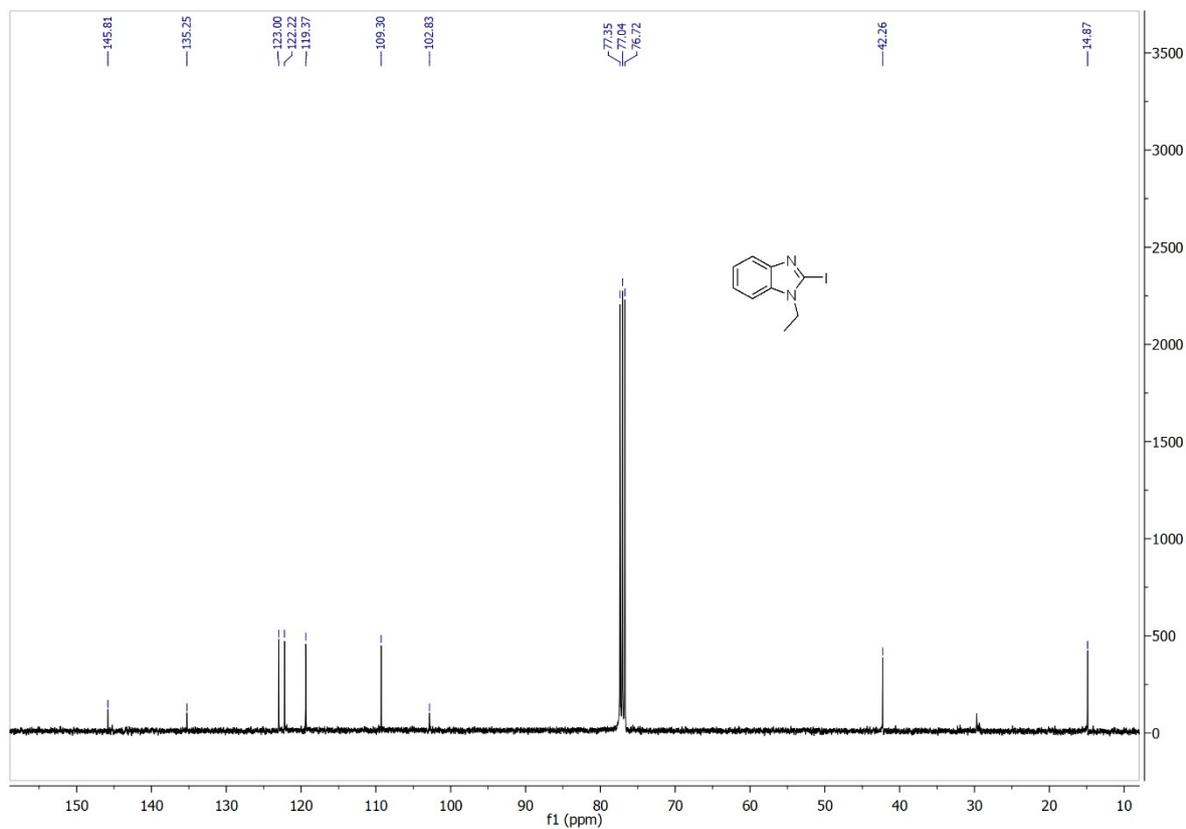
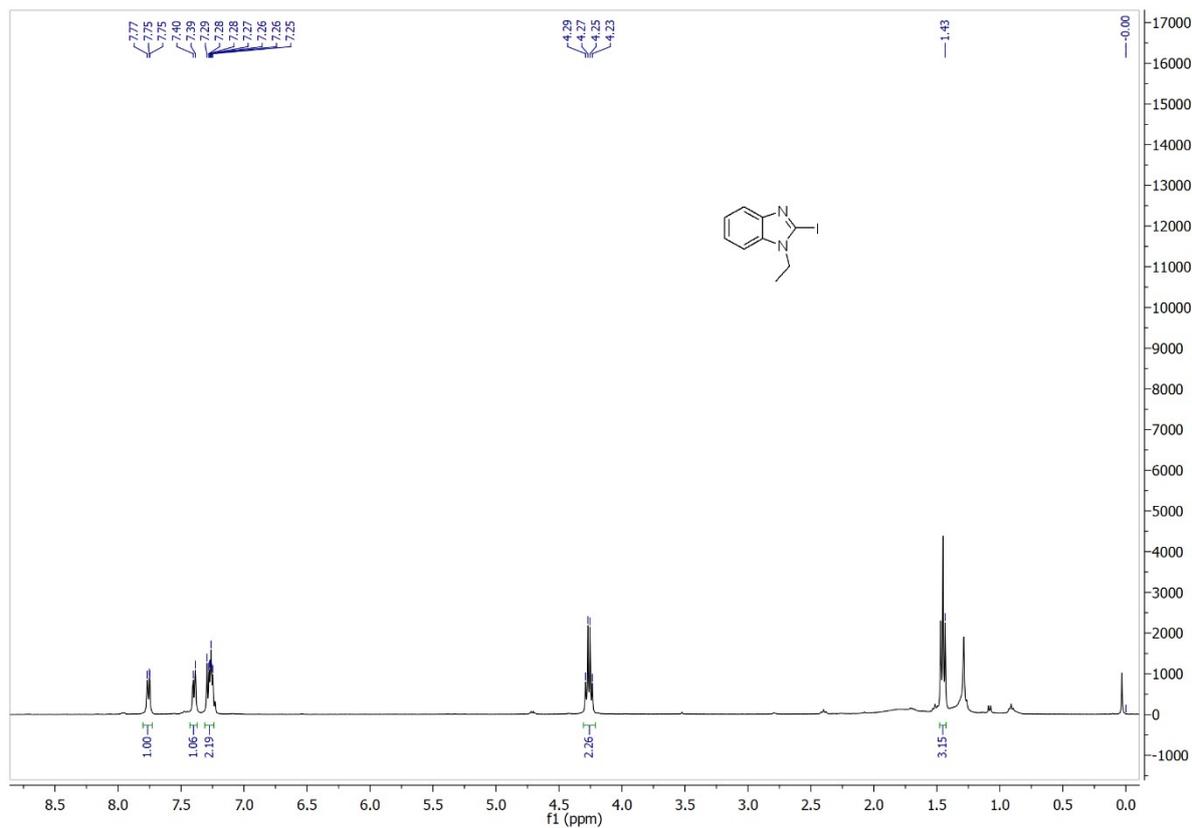
### 3-Chloro-2-(4-methoxyphenyl)benzo[d]imidazo[2,1-b]thiazole (6h):



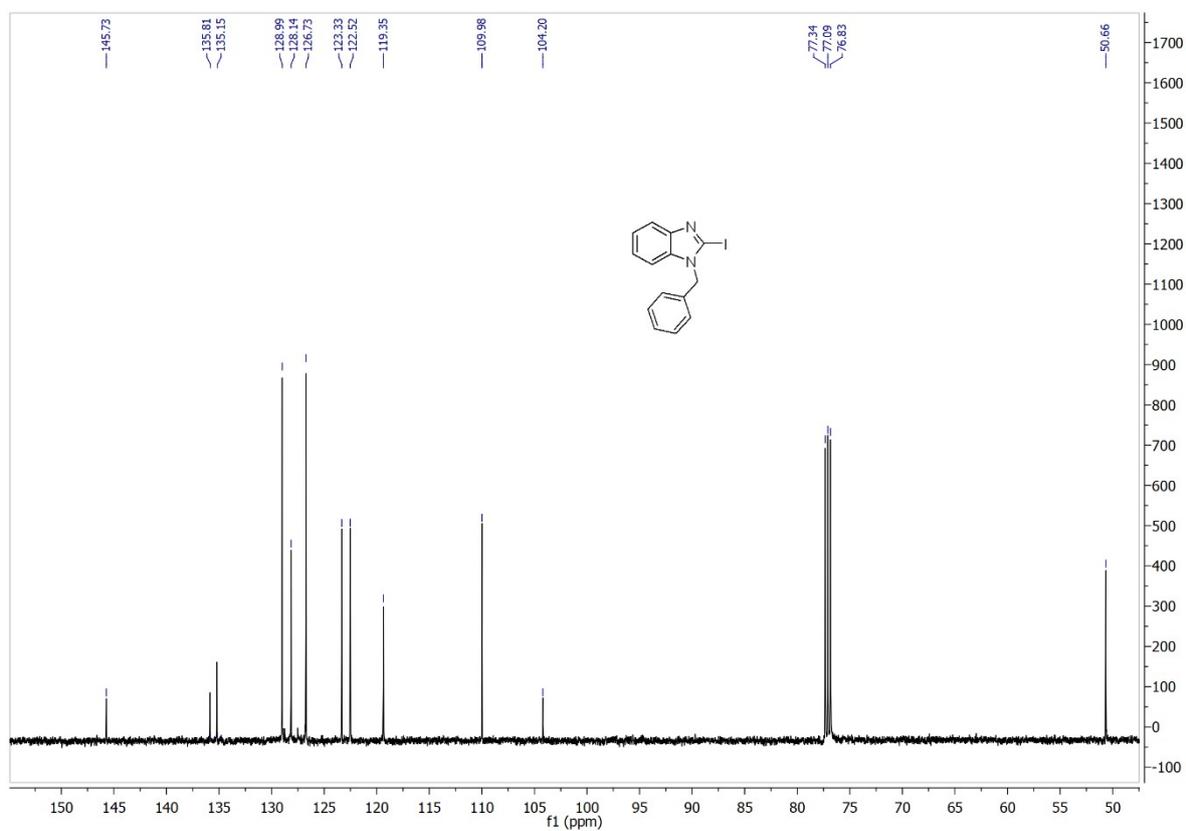
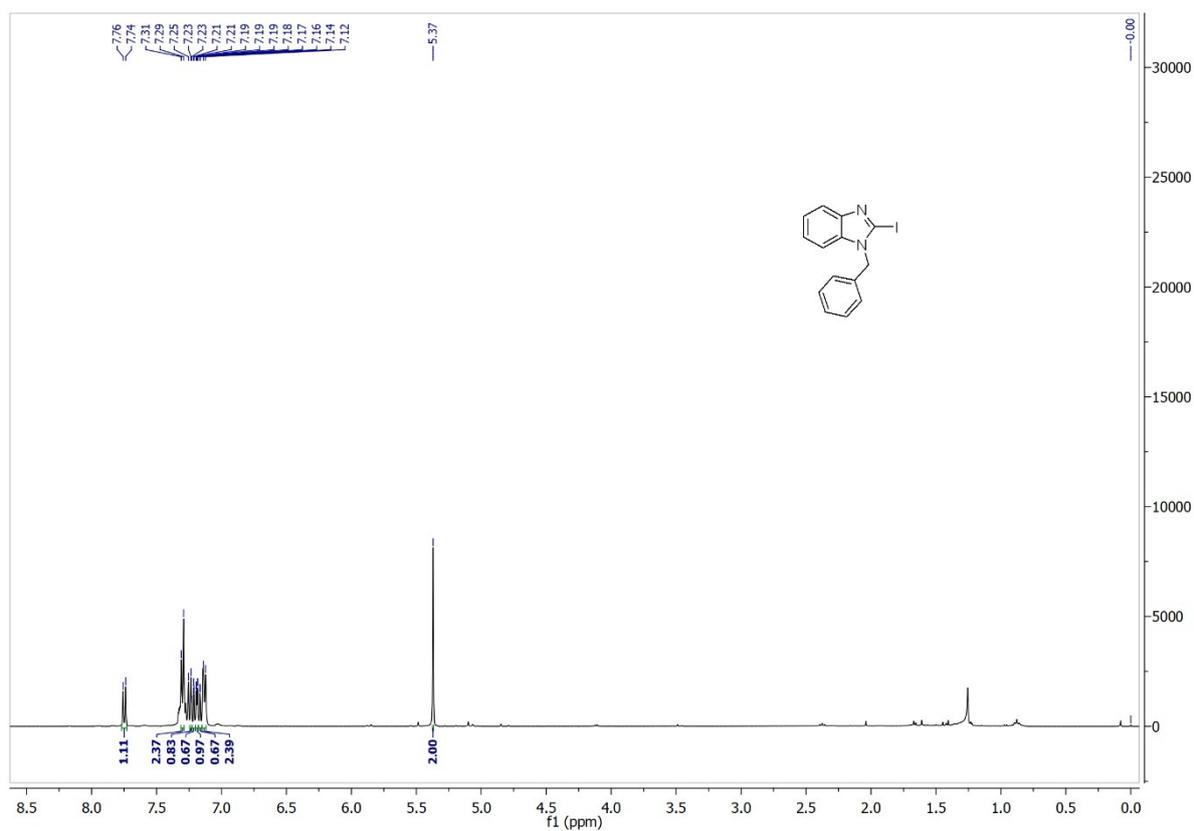
## 2-Iodo-1-methyl-1H-benzo[d]imidazole (8a)



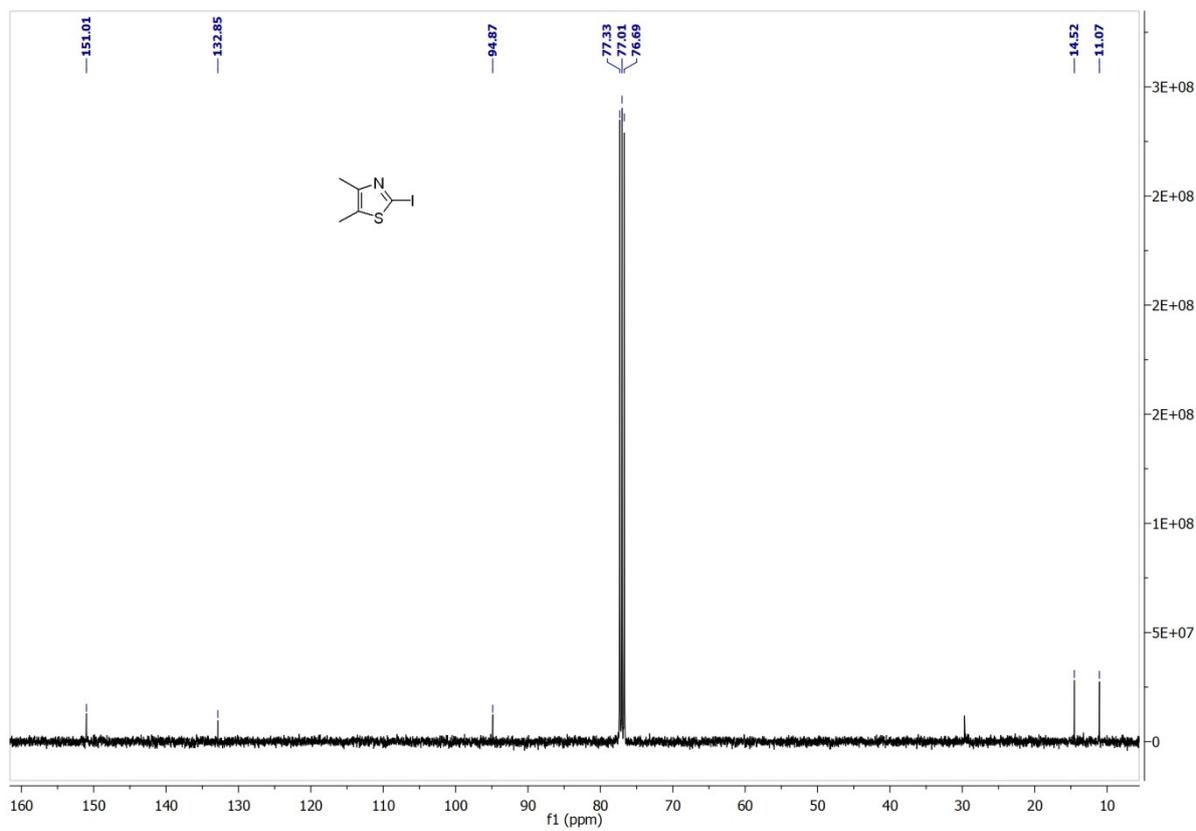
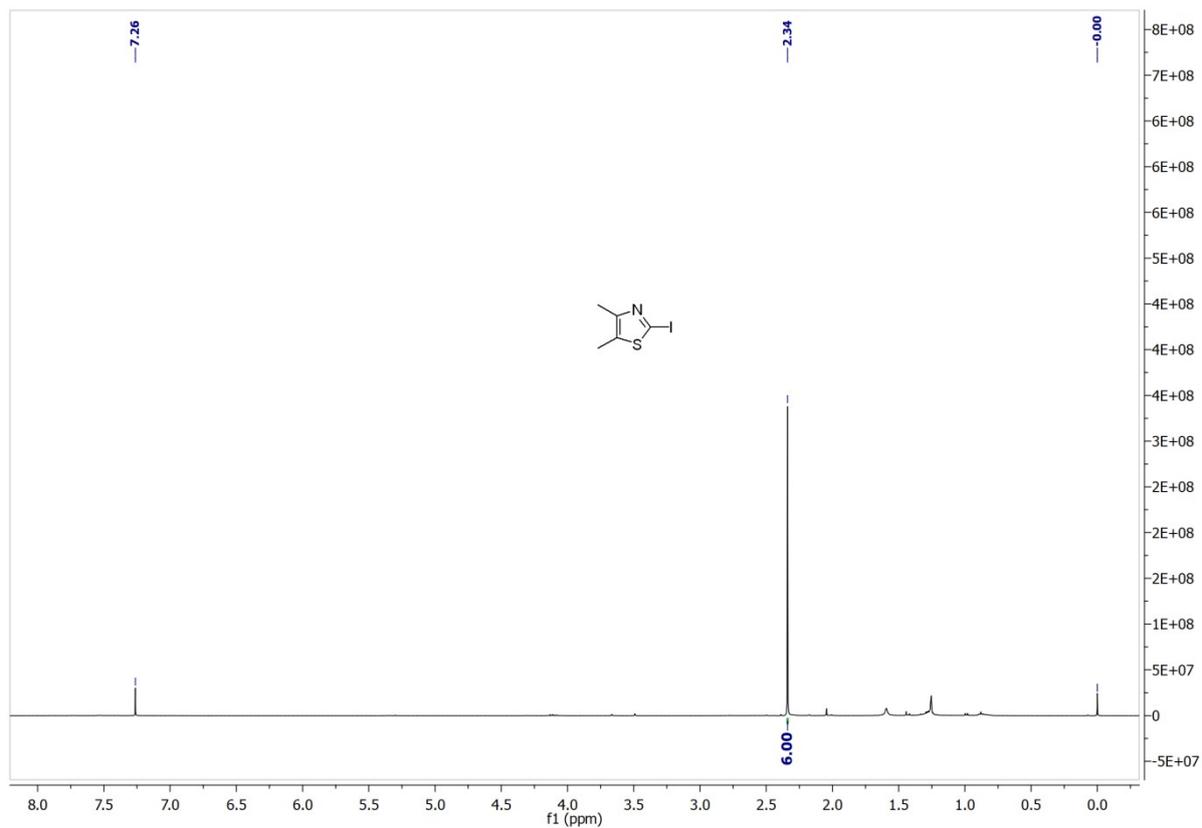
# 1-Ethyl-2-iodo-1*H*-benzo[d]imidazole (8b)



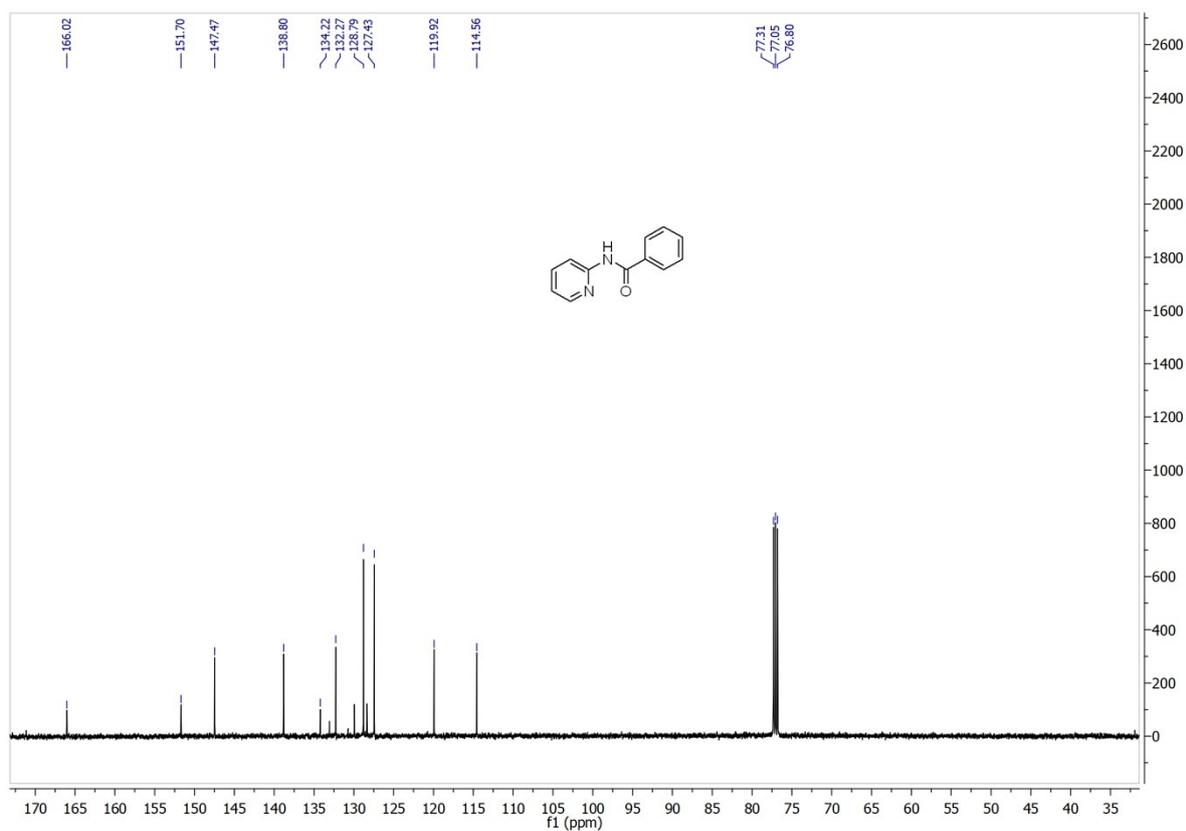
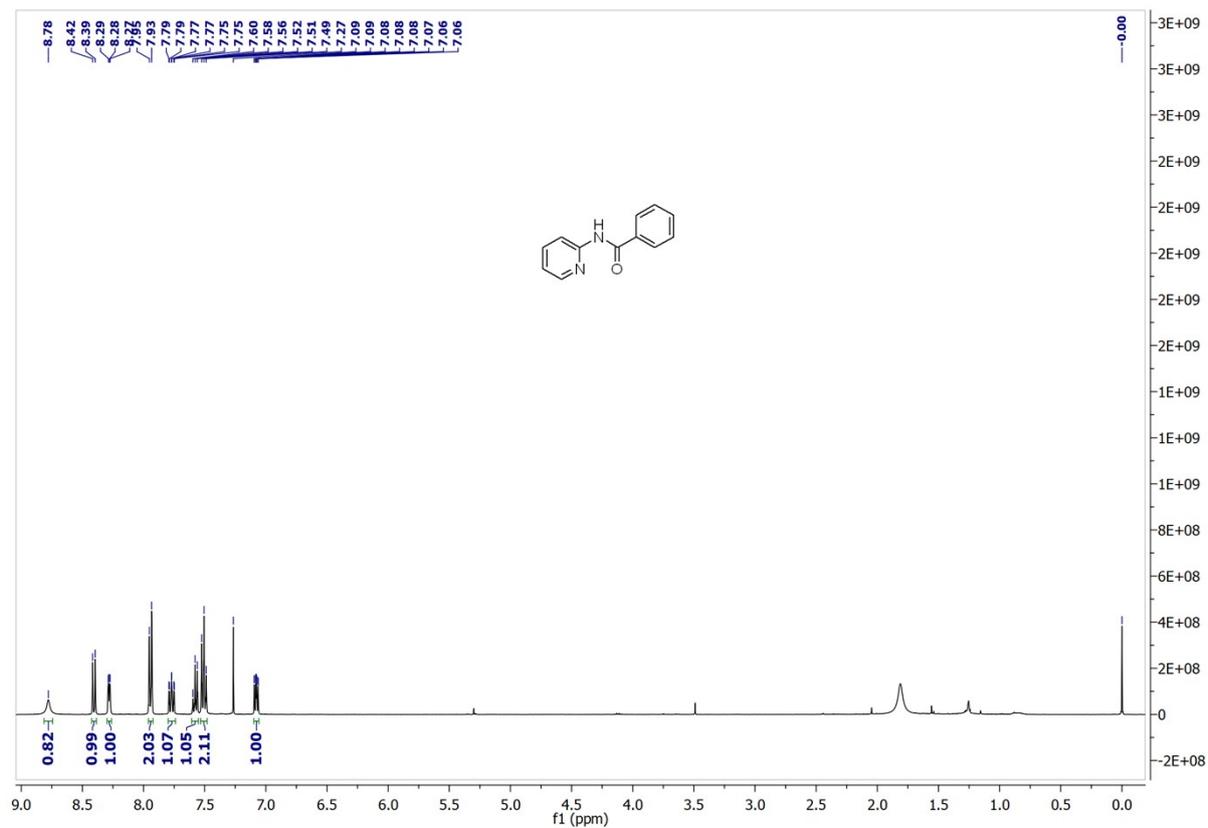
# 1-Benzyl-2-iodo-1*H*-benzo[*d*]imidazole (8c)



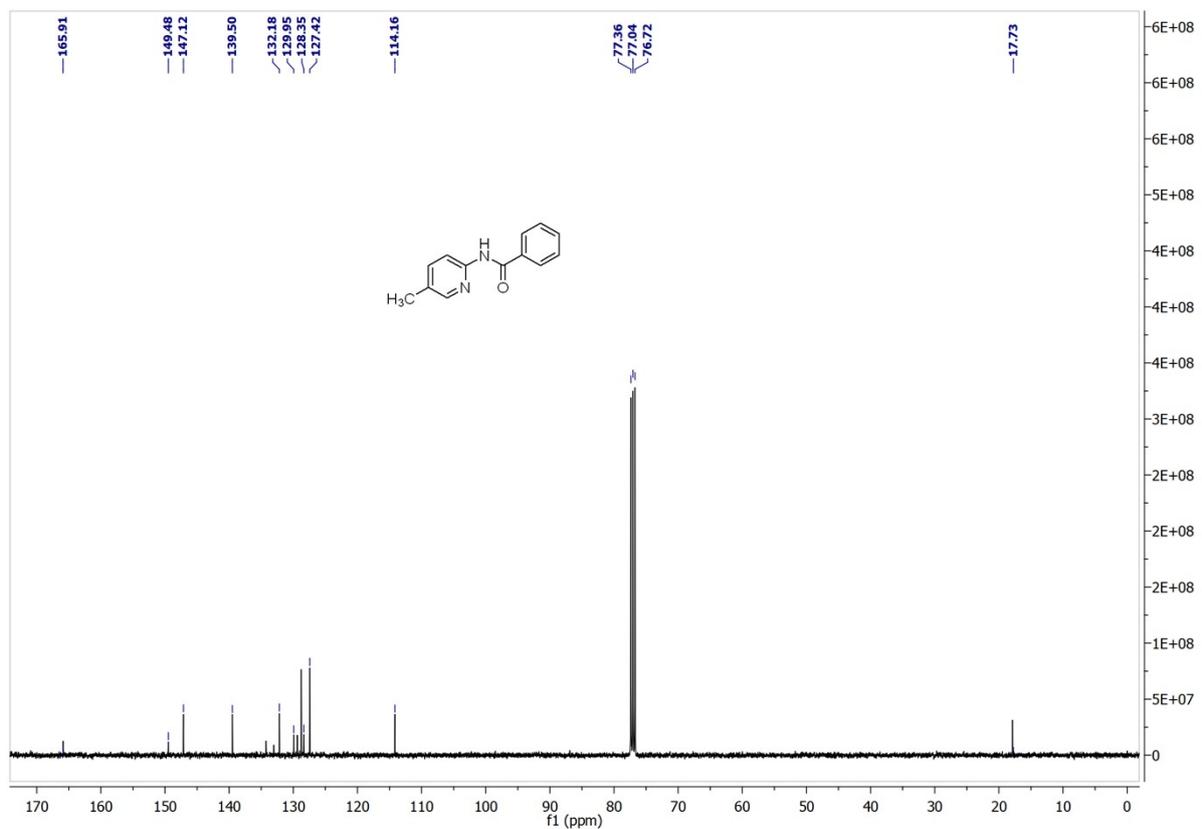
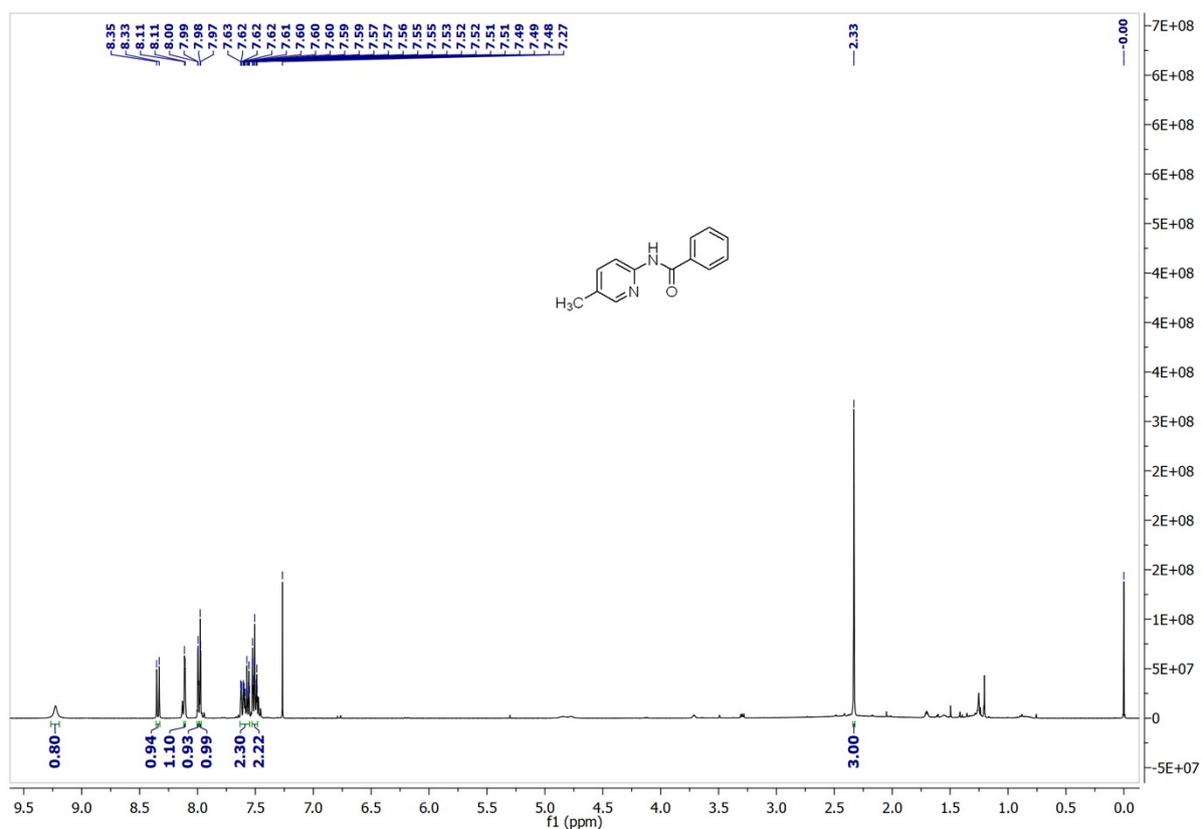
## 2-Iodo-4,5-dimethylthiazole (8e)



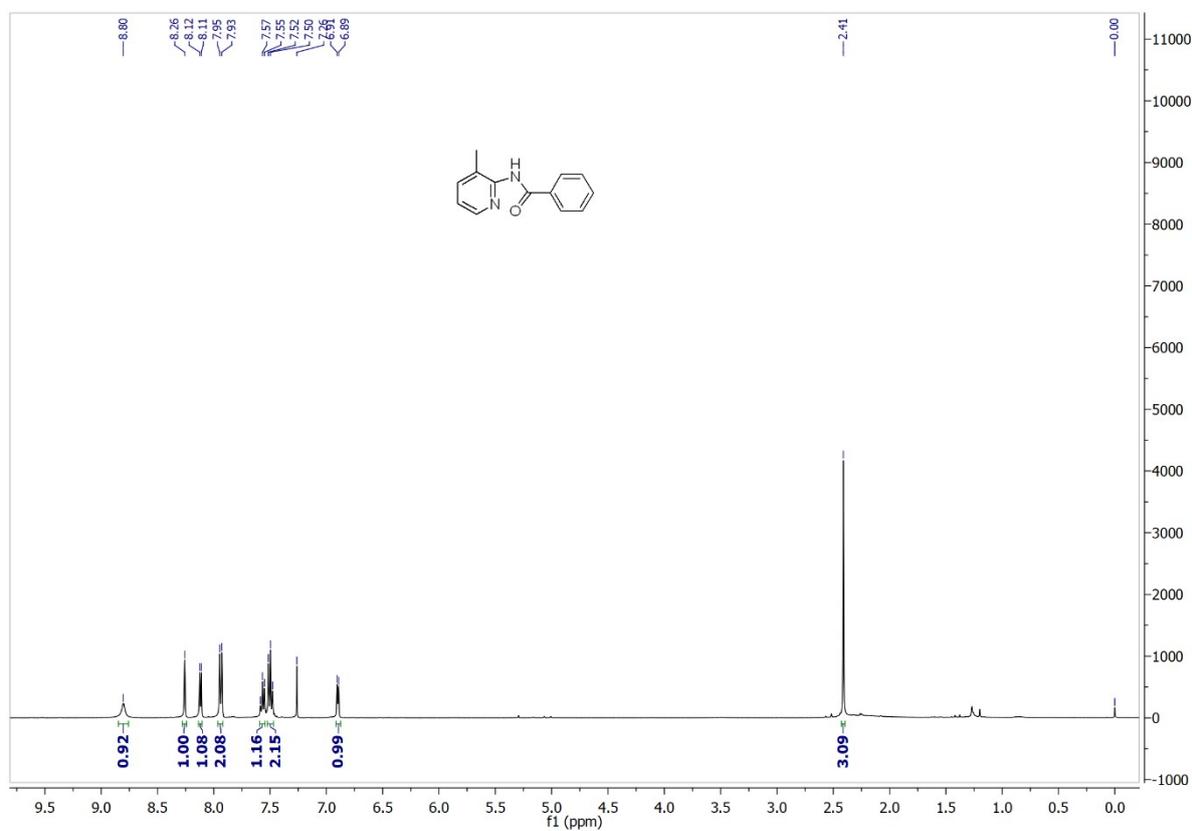
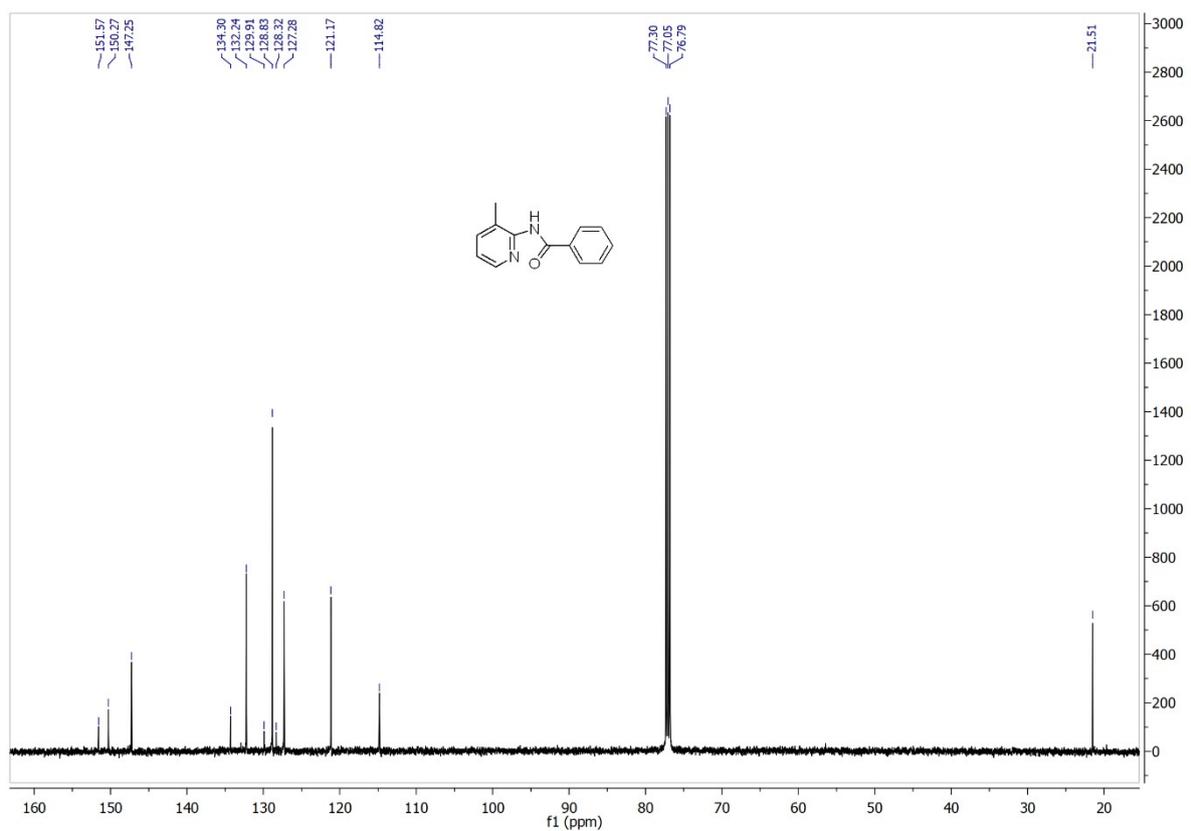
# N-(Pyridin-2-yl)benzamide (3a)



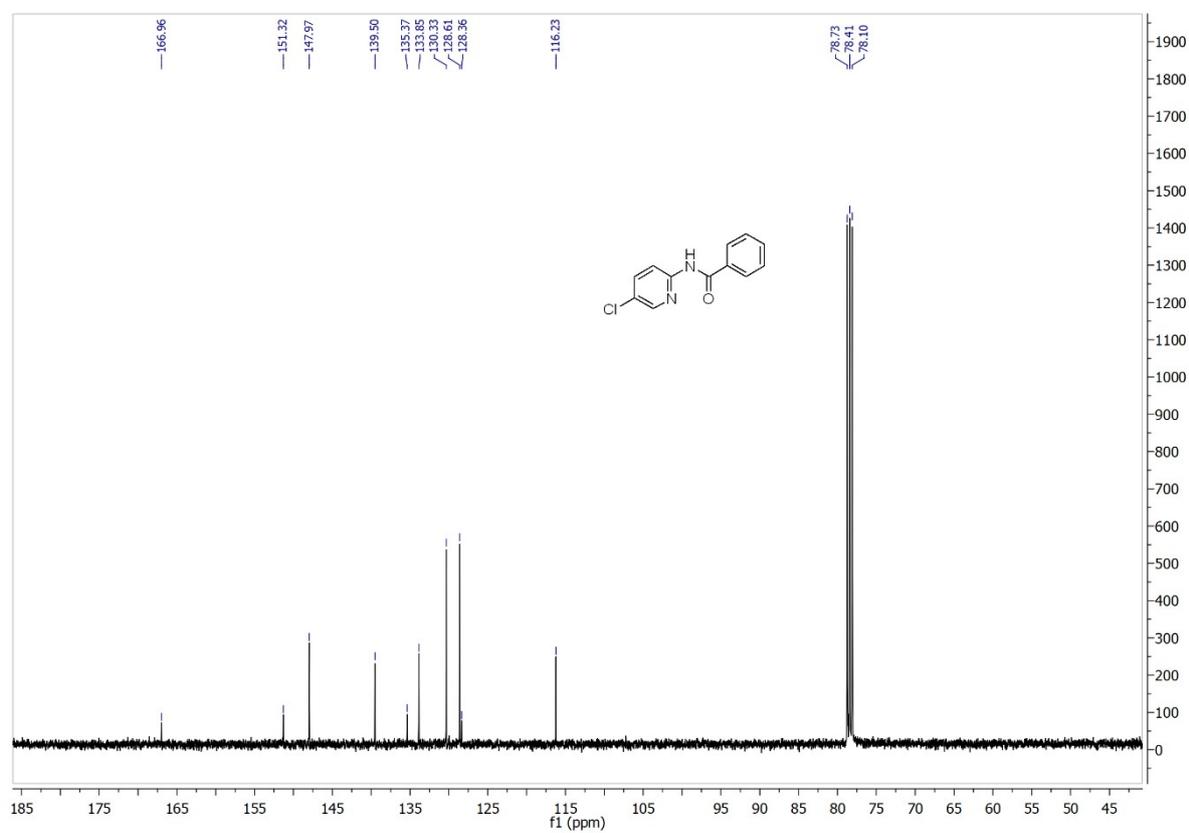
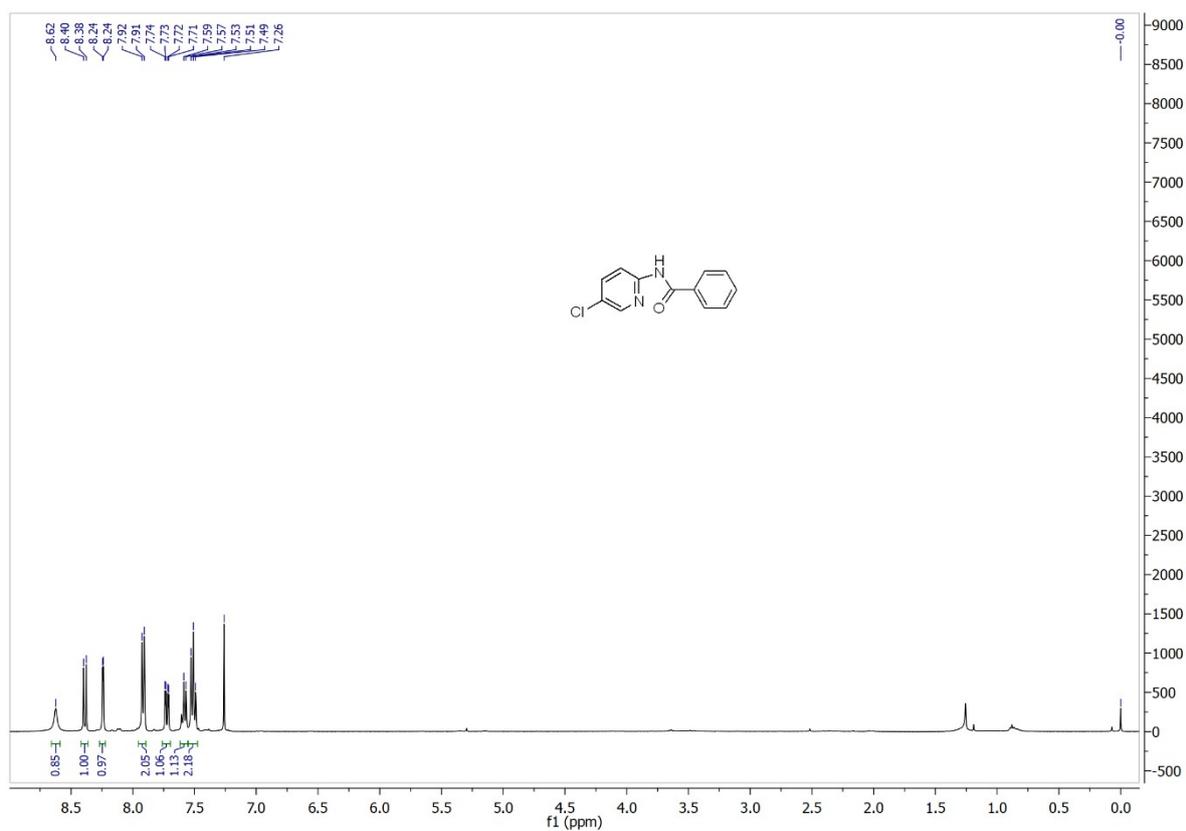
# N-(5-Methylpyridin-2-yl)benzamide (3b)



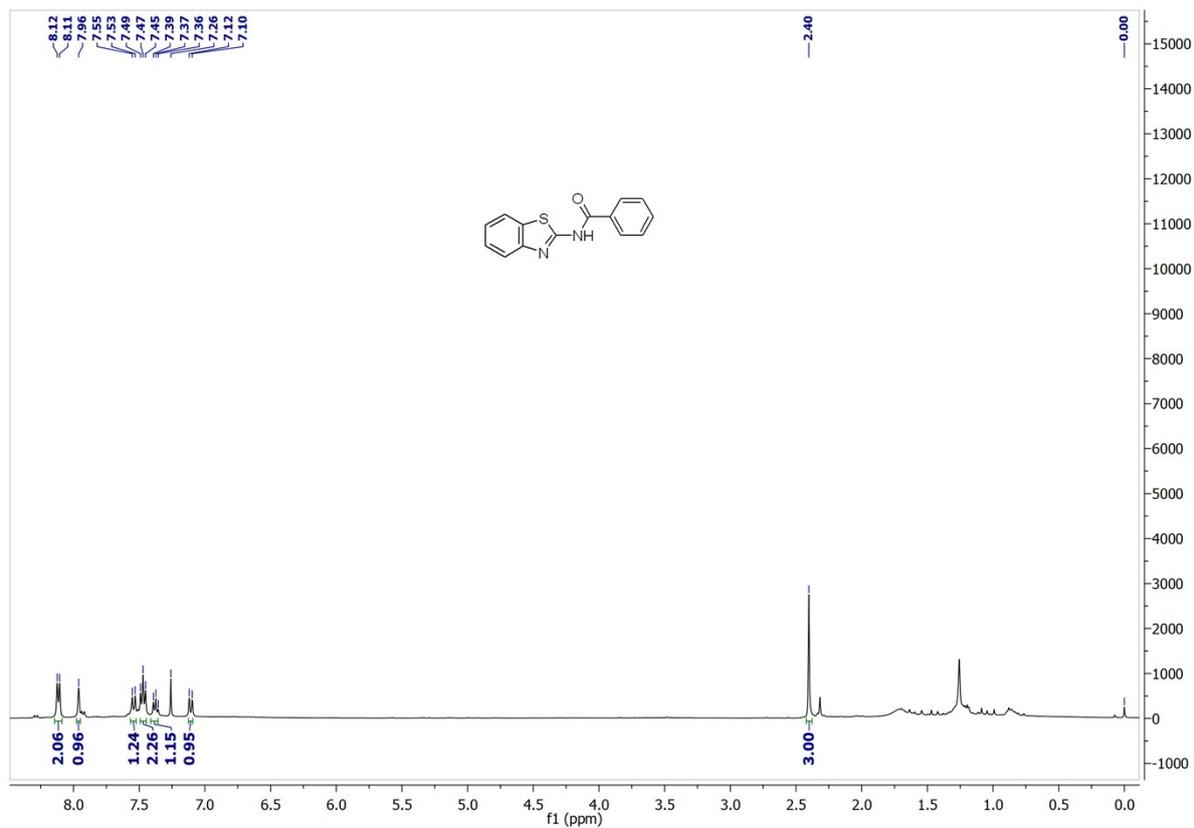
### N-(4-Methylpyridin-2-yl)benzamide (3c):



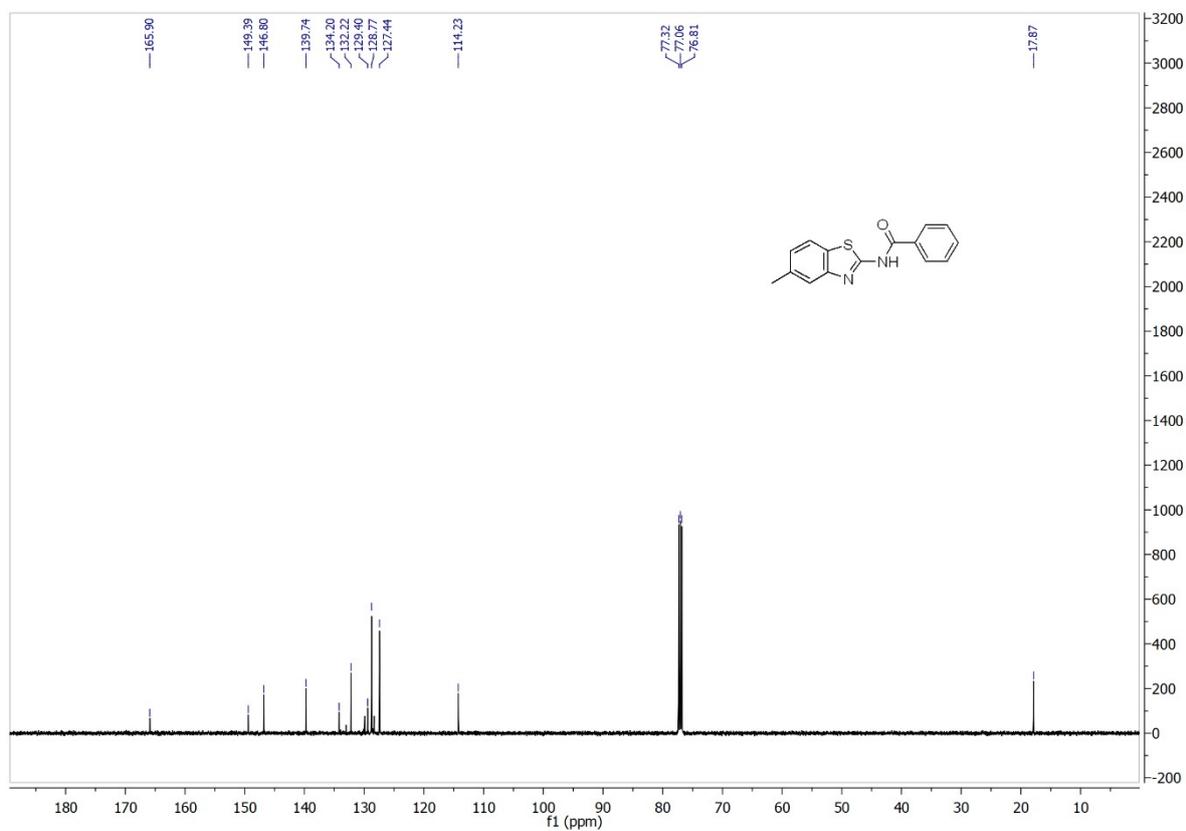
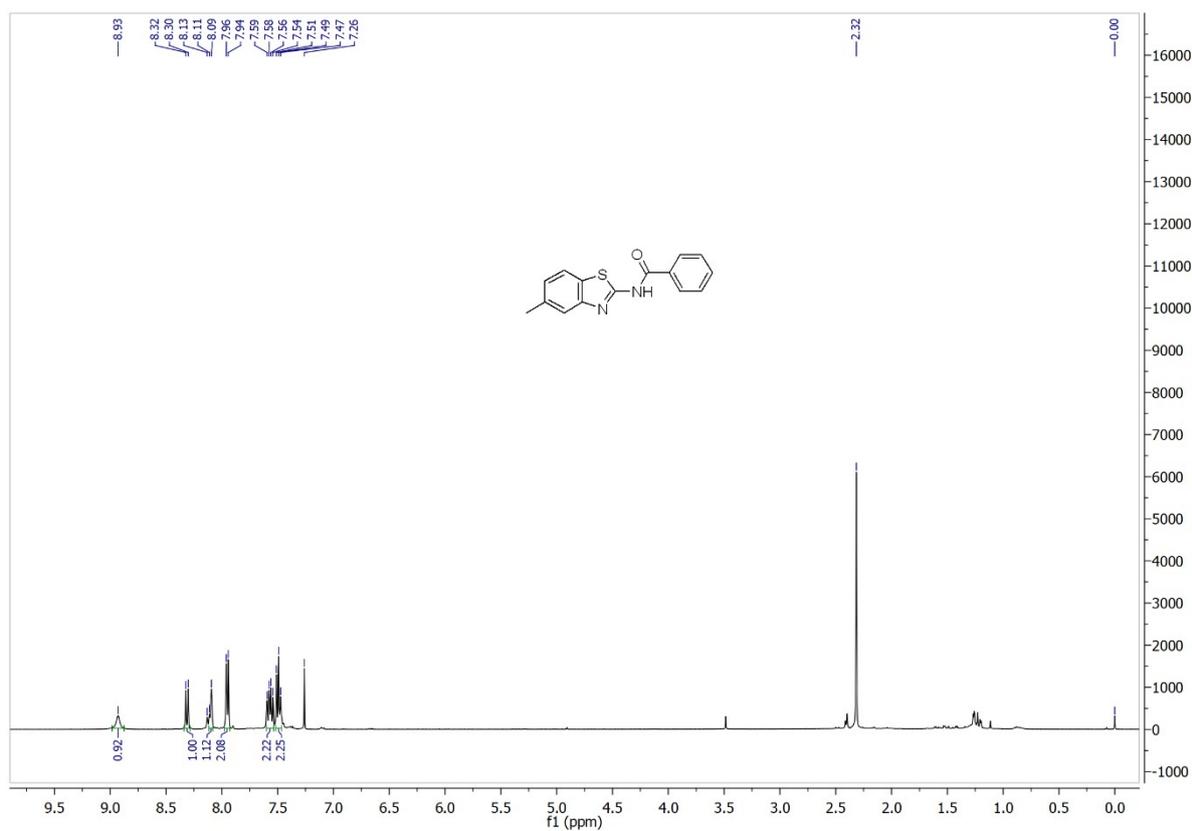
### N-(5-Chloropyridin-2-yl)benzamide (3d):



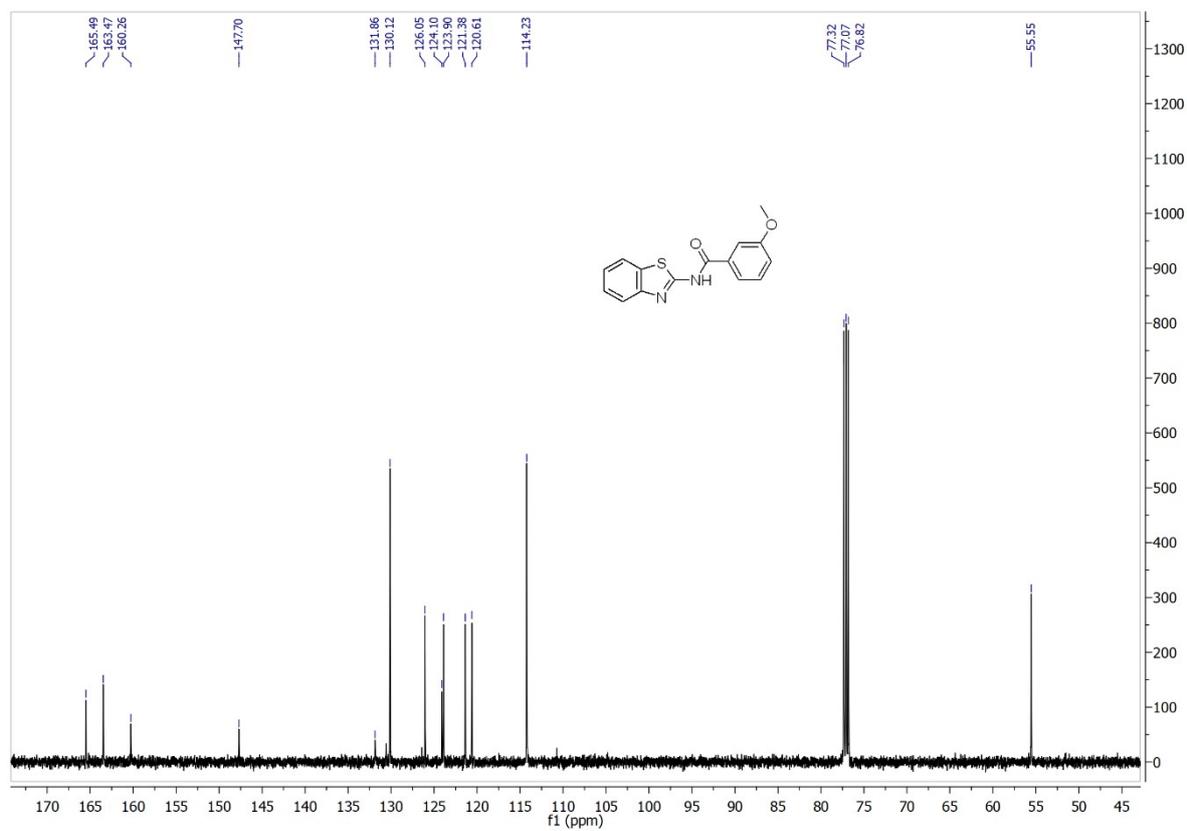
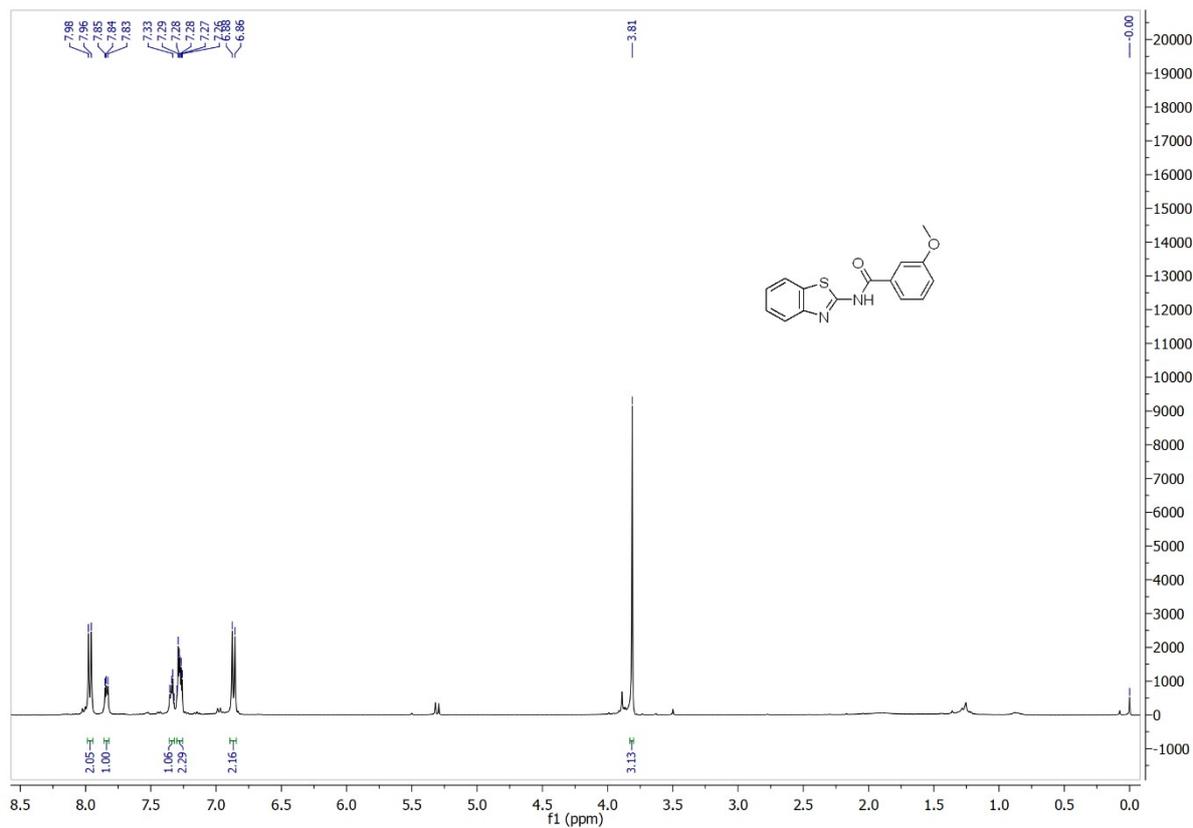
# N-(Benzo[d]thiazol-2-yl)benzamide (3e)



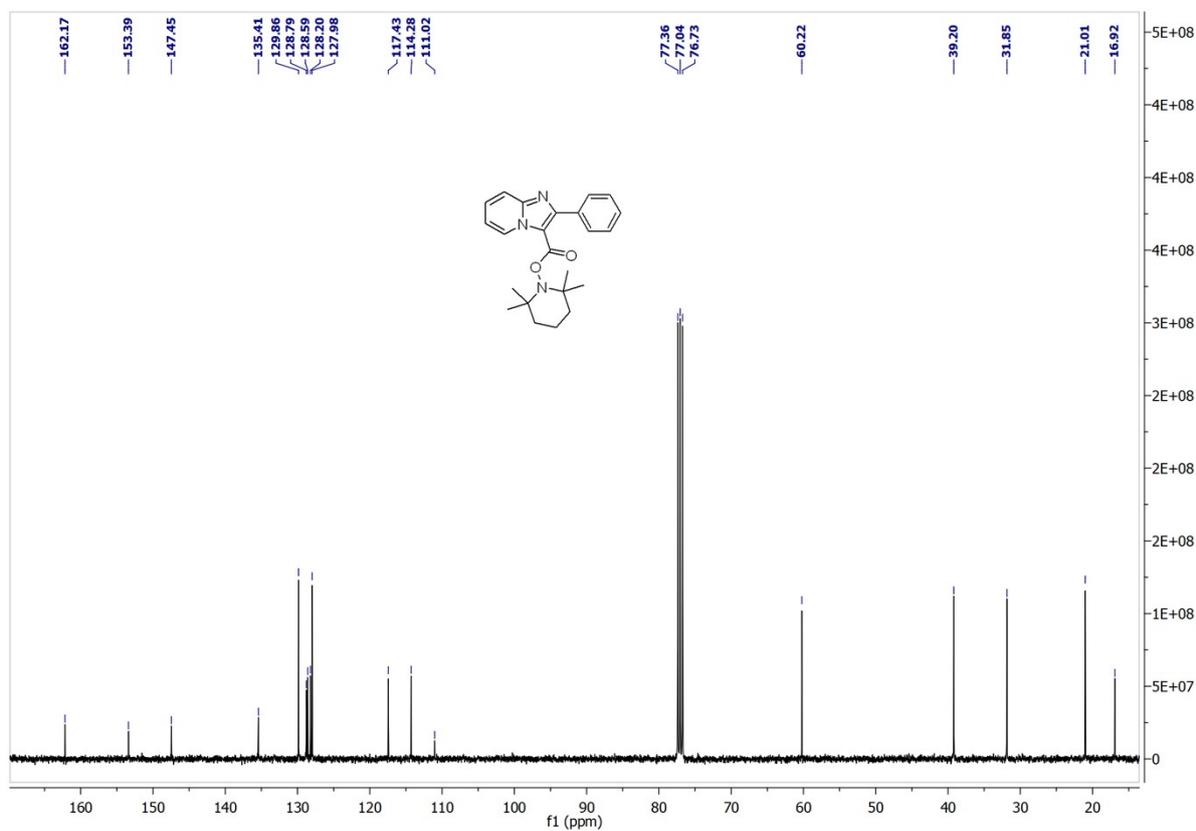
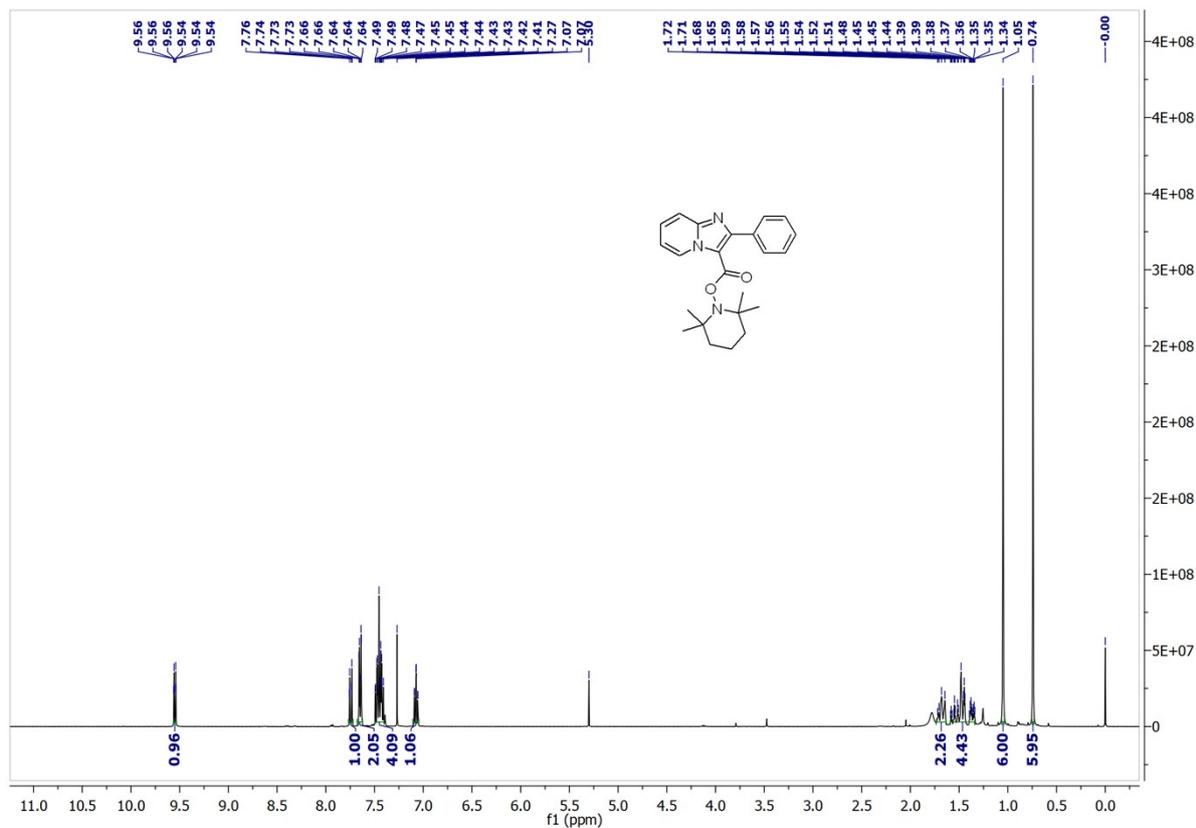
# N-(5-Methylbenzo[d]thiazol-2-yl)benzamide (3f)

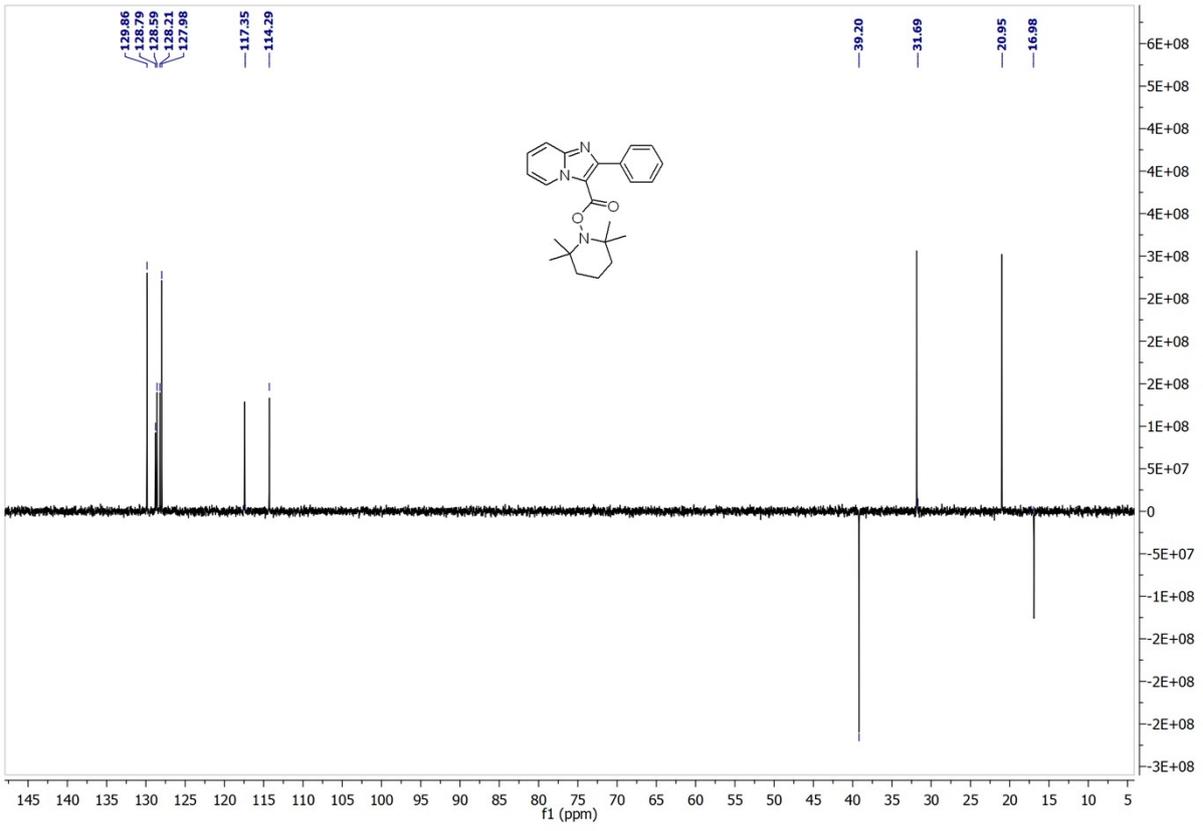


# N-(Benzo[d]thiazol-2-yl)-3-methoxybenzamide (3g)

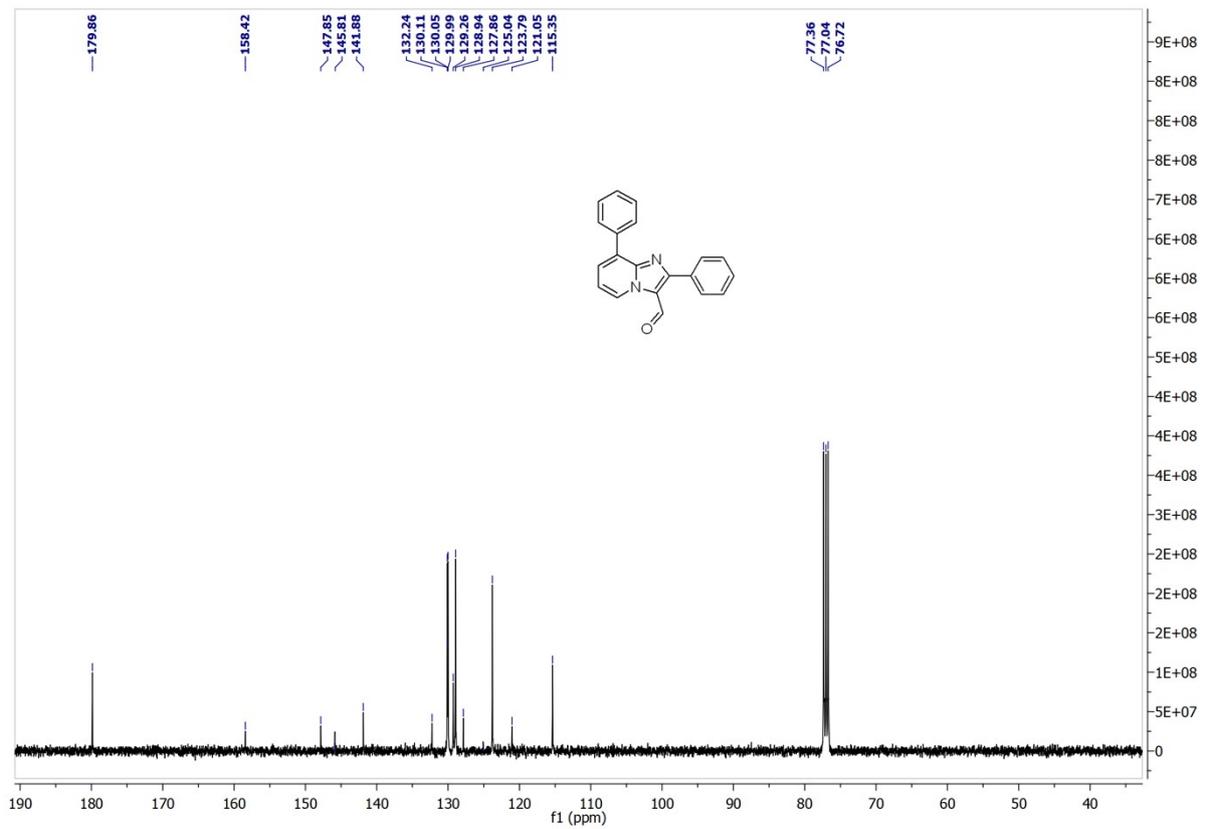
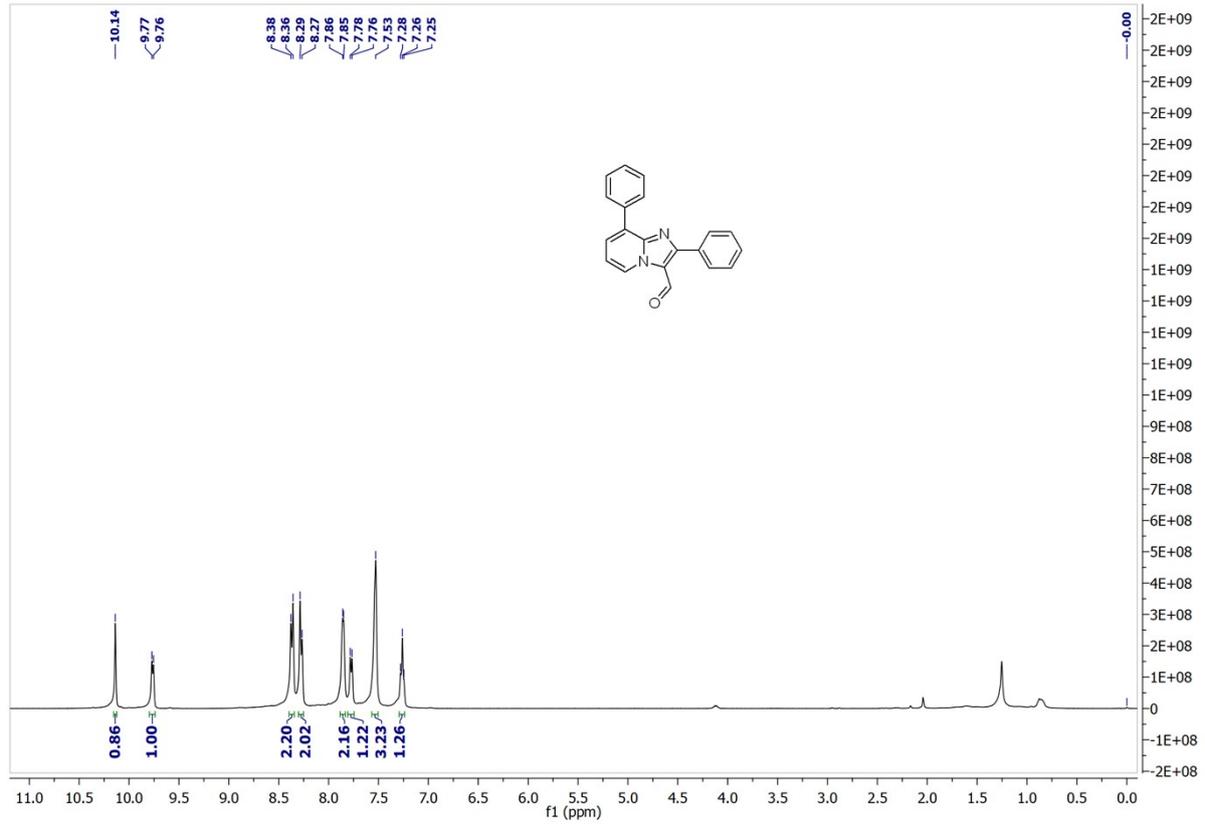


# 2,2,6,6-Tetramethylpiperidin-1-yl 2-phenylimidazo[1,2-a]pyridine-3-carboxylate (9)

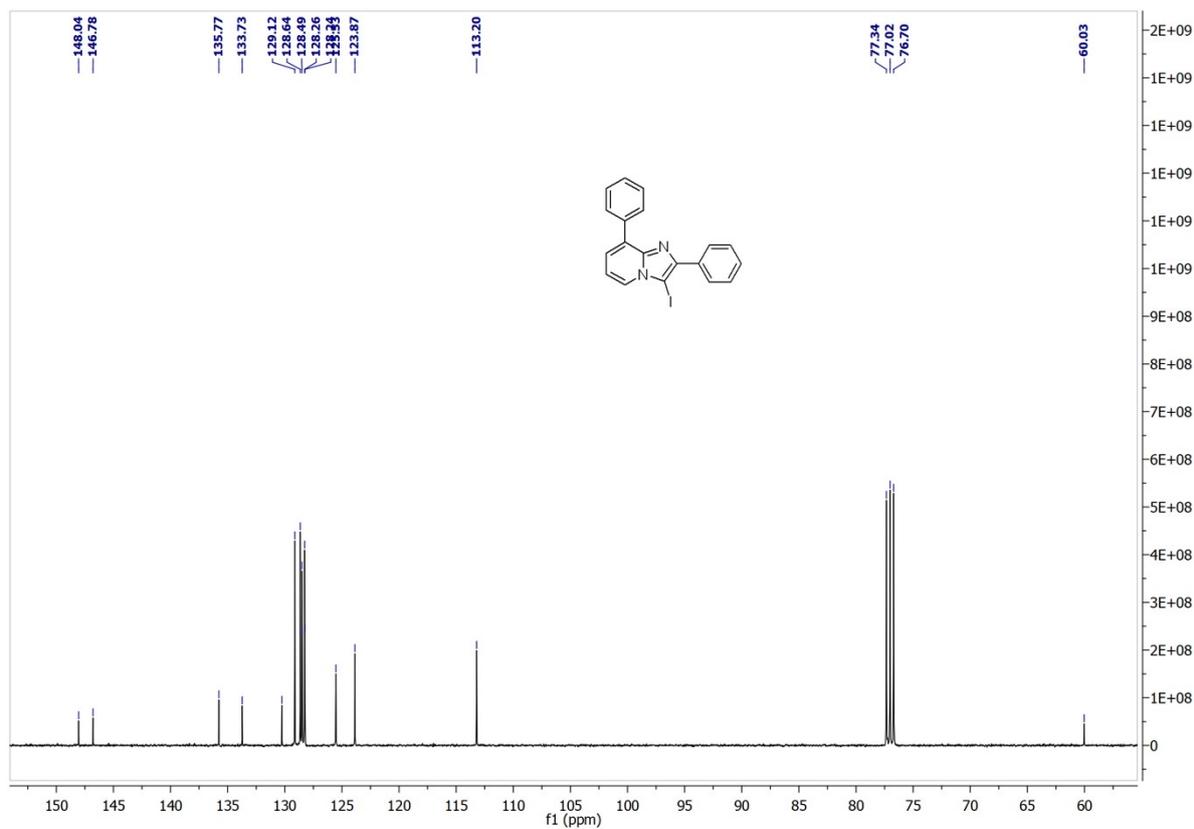
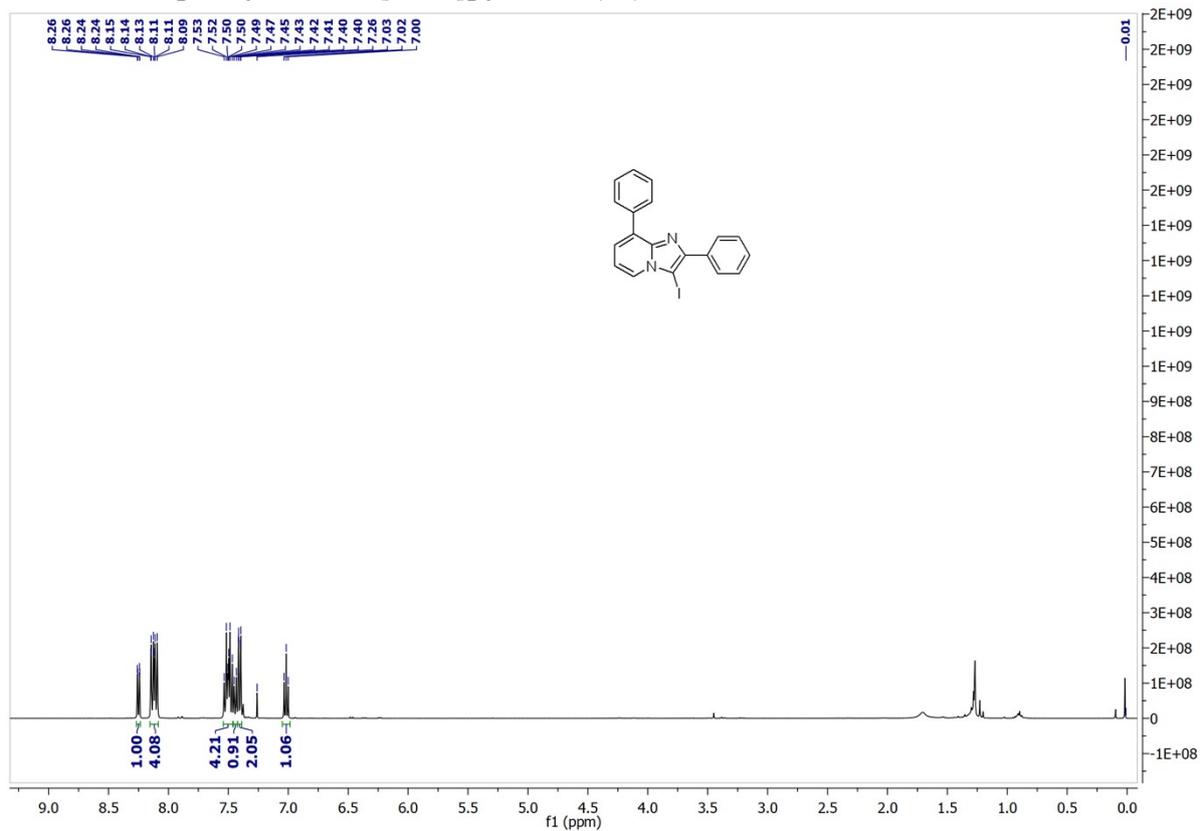




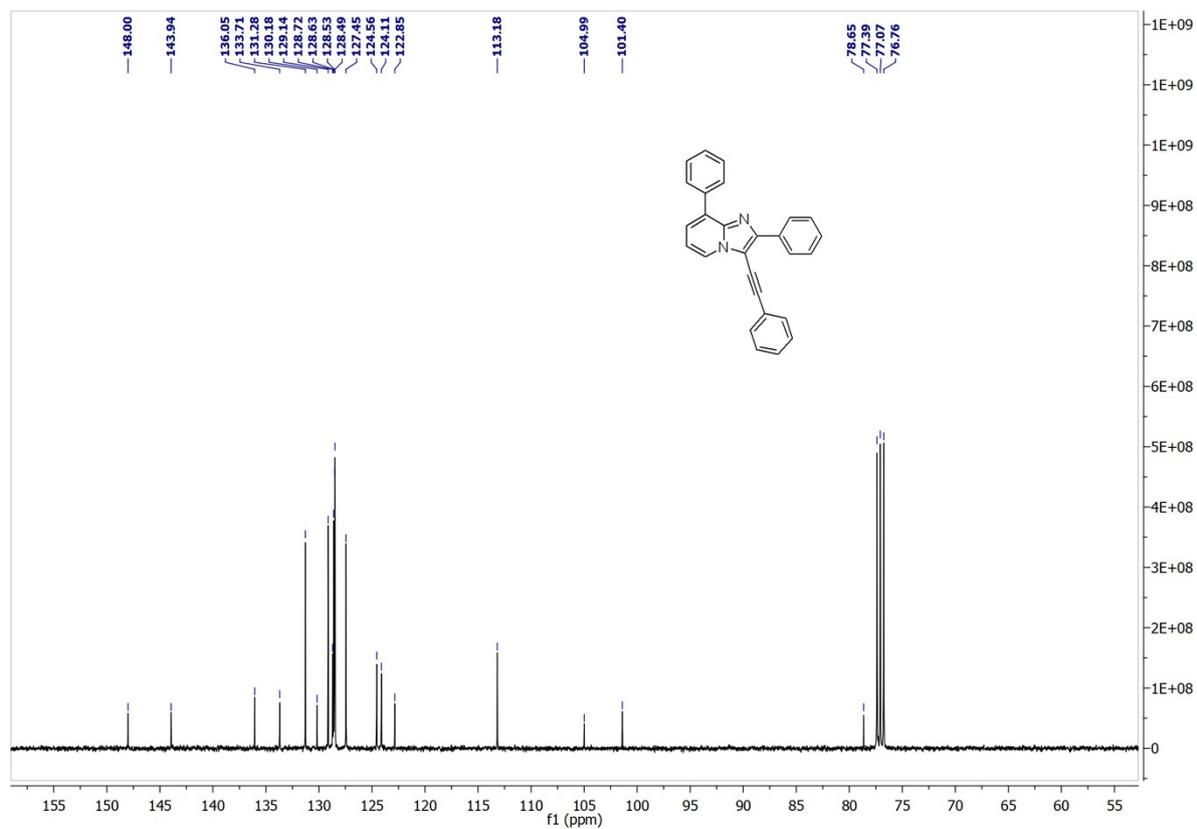
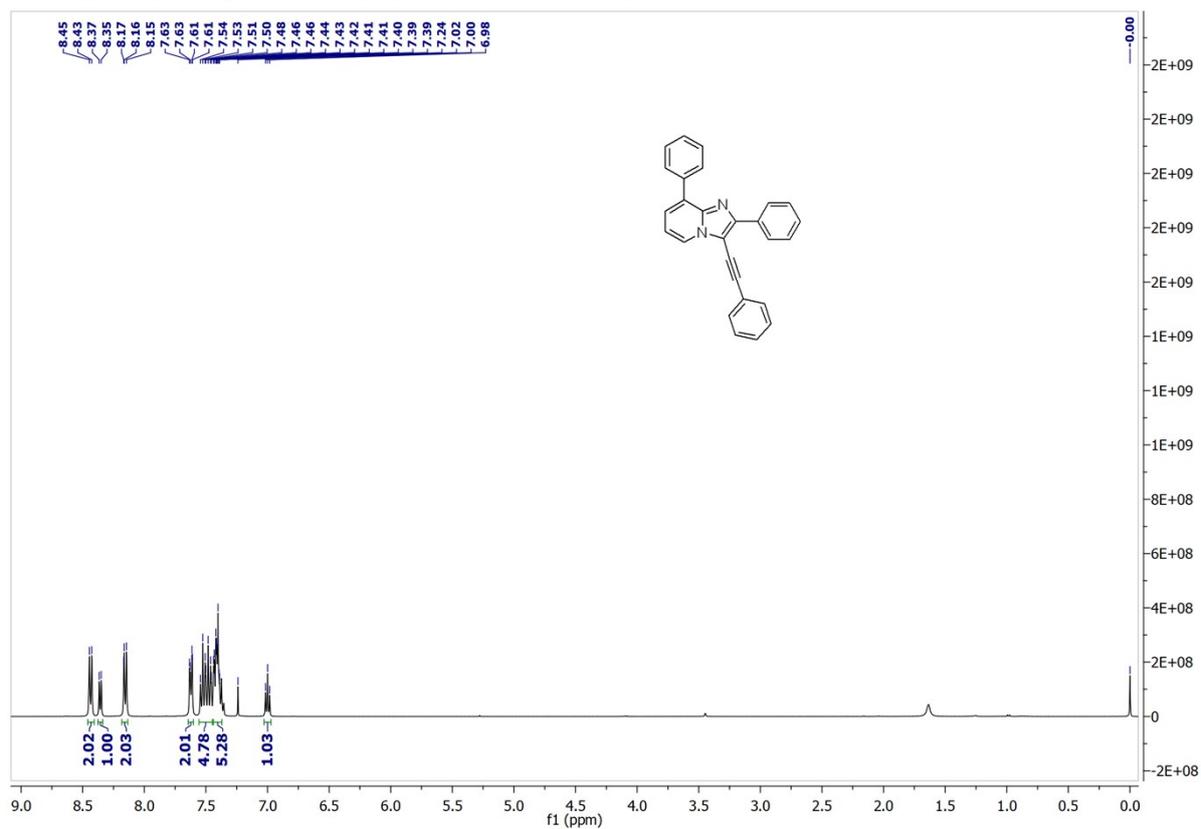
**3-Iodo-2,8-diphenylimidazo[1,2-a]pyridine (10):**



### 3-Iodo-2,8-diphenylimidazo[1,2-a]pyridine (11):



## 2,8-Diphenyl-3-(phenylethynyl)imidazo[1,2-a]pyridine (12):



## References

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